See disclosed macrocyclic compound on PCT search

L1 ANSWER 1 OF 1 WPINDEX (C) 2002 THOMSON DERWENT
Full Text
AN 1995-275891 [37] WPINDEX
DNC C1995-125128
TI New octa aza macrocyclic cpds. - useful as contrast agents in X-ray and NMR diagnostics and as radiopharmaceuticals.
DC B03 B04 K08
IN BOETTGER, U; GRIES, H; PLATZEK, J; RADUECHEL, B; SCHUMANN, H
PA (SCHD) SCHERING AG
CYC 19
PI DE 4403039 A1 19950803 (199537)* 16p C07D259-00
WO 9520580 A1 19950803 (199537) C07D259-00
RW: AT BE CH DE DK ES FR GB GR IE IT LU MC NL PT SE
W: CA JP US
ADT DE 4403039 A1 DE 1994-4403039 19940128; WO 9520580 A1 WO 1995-EP124 19950113
PRAI DE 1994-4403039 19940128
REP EP 197437; WO 9208725; WO 9312097
IC ICM C07D259-00
ICS A61K031-33; A61K049-04; A61K051-00; C07F009-6524
ICI C07M005:
AB DE 4403039 A UPAB: 19950921
Octaazamacrocyclics (I) and their salts with bases and amino acids are new: R1-R7 = H; 1-10C alkyl or aralkyl opt. substd. by 1 NH2 and/or 1-5 OH and/or opt. interrupted by O or NH; 6-12C aryl or aralkyl opt. aryl-substd. by 1 isothiocyanato or 1-3 halo; A, D, W = a gp. of formula (i); m, n = 0-2; X = -COOH; -COOM; -PO3H2; -PO3HM; -PO3M2; -PO2H-R8; OR -PO2M-R8; R8 = 1-10C alkyl or aralkyl; M = ion (opt. bonded via O) of a metal of atomic number 21-32, 37-39, 42-51 or 56-83; provided that m+n 1.

USE - (I) are useful as contrast agents in X-ray and NMR diagnostics, e.g. for the detection of tumours and cardiac infarction. (I) can also be used as radiopharmaceuticals, e.g. to destroy tumour cells in-situ. The respective formulations, which e.g. contain 0.05-2 mol/l of a Ca, Mg or Zn salt or complex in order to improve tolerance, can be administered enterally or, pref., parenterally, esp. intravenously.

ADVANTAGE - (I) produce a stronger imaging effect than cpds. known from US4647447 when used in the same concn.. Further, they are well tolerated, have high stability and a good solubility in water, with low osmolarity and favourable excretion kinetics. They also have a high relaxivity, which can be increased synergistically by incorporating 2 paramagnetic metal ions, and a high absorption coefficient for X-rays.
Dwg.0/0
FS CPI
FA AB; DCN
MC CPI: B05-B01E; B07-D13; B12-K04A1; B12-K04A2; B12-K04B; B12-K04C2; B14-H01; K08-E; K09-B; K09-E

L2 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS
Full Text
AN 1995:795167 CAPLUS
DN 123:186926
TI Octaazamacrocycles, their metal complexes, method of preparation of compounds and compositions in media and use in diagnostics and therapy
IN Schumann, Herbert; Boettger, Ulrike; Gries, Heinz; Platzek, Johannes; Raduechel, Bernd
PA Schering A.-G., Germany
SO Ger. Offen., 15 pp.
CODEN: GWXXBX
DT Patent
LA German
IC ICM C07D259-00
ICS C07F009-6524; A61K049-00; A61K051-00; A61K049-04; A61K031-33
ICA C07C229-16; C07C053-15; C07C311-18
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 28
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 4403039	A1	19950803	DE 1994-4403039	19940128
	WO 9520580	A1	19950803	WO 1995-EP124	19950113

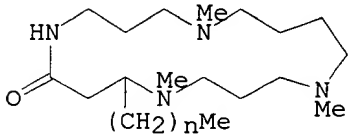
W: CA, JP, US
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

PRAI DE 1994-4403039 19940128
OS MARPAT 123:186926
AB 1,4,7,10,13,16,19,22-Octaazacyclotetracosaneoctaacetic acid and 1,4,7,10,14,17,20,23-octaazacyclohexacosaneoctaacetic acid and their Mn, Ru and lanthanide mononuclear or dinuclear complexes were prepd.
ST octaazacyclotetracosaneoctaacetic acid prepn complexation; octaazacyclohexacosaneoctaacetic acid prepn complexation; lanthanide octaaza macrocycle acetato complex; manganese octaaza macrocycle acetato complex; ruthenium octaaza macrocycle acetato complex; macrocycle octaaza acetato transition metal complex
IT Transition metal compounds
RL: SPN (Synthetic preparation); PREP (Preparation)
(octaaza macrocycle octaacetic acid complexes)
IT 627-18-9, 3-Bromo-1-propanol 25512-65-6, Dihydropyran
RL: RCT (Reactant); RACT (Reactant or reagent)
(for prepn. of octaazacyclohexacosaneoctaacetic acid and its transition metal complexes)
IT 33821-94-2P 163164-92-9P 167861-79-2P 167861-80-5P 167861-83-8P 167861-84-9P 167861-85-0P 167861-86-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for prepn. of octaazacyclohexacosaneoctaacetic acid and its transition metal complexes)
IT 297-11-0 5292-43-3, tert-Butyl bromoacetate
RL: RCT (Reactant); RACT (Reactant or reagent)
(for prepn. of octaazacyclotetracosaneoctaacetic acid and its transition metal complexes)
IT 167861-81-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for prepn. of octaazacyclotetracosaneoctaacetic acid and transition metal complexes)
IT 167861-82-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(prepn. and complexation with transition metals)

IT 7439-96-5DP, Manganese, octaaza macrocycle octaacetic acid complexes
7440-18-8DP, Ruthenium, octaaza macrocycle octaacetic acid complexes
7440-19-9DP, Samarium, octaaza macrocycle octaacetic acid complexes
7440-53-1DP, Europium, octaaza macrocycle octaacetic acid complexes
7440-54-2DP, Gadolinium, octaaza macrocycle octaacetic acid complexes
7440-64-4DP, Ytterbium, octaaza macrocycle octaacetic acid complexes
16833-27-5DP, Oxide, transition metal octaaza macrocycle octaacetic acid complexes 163164-92-9DP, transition metal complexes 167861-82-7DP, transition metal complexes
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

AN 1992:207412 CAPLUS
DN 116:207412
TI Biological activity of novel macrocyclic alkaloids (budmunchiamines) from Albizia amara detected on the basis of interaction with DNA
AU Mar, Woongchon; Tan, Ghee T.; Cordell, Geoffrey A.; Pezzuto, John M.; Jurcic, Ksenija; Offermann, Franziska; Redl, Karl; Steinke, Bernice; Wagner, Hildebert
CS Coll. Pharm, Univ. Illinois, Chicago, IL, 60612, USA
SO Journal of Natural Products (1991), 54(6), 1531-42
CODEN: JNPRDF; ISSN: 0163-3864
DT Journal
LA English
CC 1-6 (Pharmacology)
GI



I, n=10
II, n=8
III, n=12

AB Exts. derived from A. amara were found to demonstrate activity in a recently developed HPLC system designed to detect compds. capable of interacting with DNA. Further investigation led to the procurement of four sets of alkaloid isolates X1-X4 that were found to be macrocyclic pithecolobine alkaloids. Isolate X1 has been identified as a mixt. of budmunchiamines A, B, and C (I, II, and III) in the ratio 4:4:1. All four isolates interacted with calf thymus DNA and were generally cytotoxic with a battery of cultured mammalian cells. As detd. with Salmonella typhimurium strain TM677, isolates X1 and X3 were bactericidal, but not mutagenic. Isolate X1 was found to inhibit the catalytic activity of DNA polymerase, RNA polymerase, and **HIV**-1 reverse transcriptase. With DNA polymerase, the reaction was shown to be inhibited in a manner that was competitive with respect to DNA. In addn., isolate X1 inhibited each of the following: platelet aggregation, human lymphocyte transformation, phorbol-ester-induced chemiluminescence with human granulocytes, and cyclooxygenase activity. Detection of these alkaloids on the basis of their interaction with DNA exemplifies the validity of this approach.

ST Albizia pithecolobine alkaloid budmunchiamine DNA pharmacol

IT Albizia amara
(alkaloids of, budmunchiamines-contg., DNA-interaction as index for isolation of, pharmacol. of)

IT Antibiotics
Blood platelet aggregation inhibitors
Inflammation inhibitors
Mutagens
Neoplasm inhibitors
(budmunchiamines-contg. alkaloids from Albizia amara as, DNA-interaction as index for isolation of)

IT Deoxyribonucleic acids
RL: BIOL (Biological study)
(interaction with, as index for isolation of budmunchiamines-contg. alkaloids from Albizia amara, pharmacol. of)

IT Alkaloids, biological studies
RL: BIOL (Biological study)
(of Albizia amara, budmunchiamines-contg., DNA-interaction as index for

isolation of, pharmacol. of)

IT Luminescence, chemi-
(with human granulocyte, budmunchiamines-contg. alkaloids from Albizia amara effect on, DNA-interaction as index of, antiinflammatory action in relation to)

IT Leukocyte
(granulocyte, chemiluminescence with human, budmunchiamines-contg. alkaloids from Albizia amara effect on, DNA-interaction as index of, antiinflammatory action in relation to)

IT Virus, animal
(human immunodeficiency 1, reverse transcriptase of, budmunchiamines-contg. alkaloids from Albizia amara effect on, DNA-interaction as index of)

IT 9012-90-2, DNA polymerase 9014-24-8, RNA polymerase
RL: BIOL (Biological study)
(budmunchiamines-contg. alkaloids from Albizia amara effect on, DNA-interaction as index of)

IT 39391-18-9, Cyclooxygenase
RL: BIOL (Biological study)
(budmunchiamines-contg. alkaloids from Albizia amara effect on, DNA-interaction as index of, anti-inflammatory action in relation to)

IT 9068-38-6, Reverse transcriptase
RL: BIOL (Biological study)
(of **HIV**-1, budmunchiamines-contg. alkaloids from Albizia amara effect on, DNA-interaction as index of)

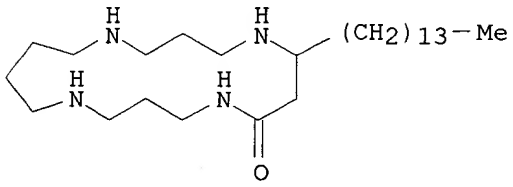
IT **139750-76-8**, Budmunchiamine A **139750-77-9**, Budmunchiamine B **139750-78-0**, Budmunchiamine C
RL: BIOL (Biological study)
(Albizia amara alkaloids contg., DNA-interaction as index for isolation of, pharmacol. of)

=>

L11 ANSWER 13 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 165467-47-0 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 8-tetradecyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine L 2**
MF C27 H56 N4 O
SR CA
LC STN Files: CA, CAPLUS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C13N4	NC3NC3NC3NC4	17	C13N4	4584.21.2	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1	pH 1	(1) ACD
Bioconc. Factor (BCF)	1	pH 4	(1) ACD
Bioconc. Factor (BCF)	1	pH 7	(1) ACD
Bioconc. Factor (BCF)	1	pH 8	(1) ACD
Bioconc. Factor (BCF)	1893	pH 10	(1) ACD
Boiling Point (BP)	611.2+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	90.76+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	132.6+/-57.0 deg C		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	4		(1) ACD
Koc (KOC)	1	pH 1	(1) ACD
Koc (KOC)	1	pH 4	(1) ACD
Koc (KOC)	1	pH 7	(1) ACD
Koc (KOC)	1	pH 8	(1) ACD
Koc (KOC)	2878	pH 10	(1) ACD
logD (LOGD)	0.59	pH 1	(1) ACD
logD (LOGD)	0.60	pH 4	(1) ACD
logD (LOGD)	0.63	pH 7	(1) ACD
logD (LOGD)	1.01	pH 8	(1) ACD
logD (LOGD)	5.09	pH 10	(1) ACD
logP (LOGP)	6.598+/-0.417		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD

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NEWS 2	Apr 08	"Ask CAS" for self-help around the clock
NEWS 3	Apr 09	BEILSTEIN: Reload and Implementation of a New Subject Area
NEWS 4	Apr 09	ZDB will be removed from STN
NEWS 5	Apr 19	US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
NEWS 6	Apr 22	Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
NEWS 7	Apr 22	BIOSIS Gene Names now available in TOXCENTER
NEWS 8	Apr 22	Federal Research in Progress (FEDRIP) now available
NEWS 9	Jun 03	New e-mail delivery for search results now available
NEWS 10	Jun 10	MEDLINE Reload
NEWS 11	Jun 10	PCTFULL has been reloaded
NEWS 12	Jul 02	FOREGE no longer contains STANDARDS file segment
NEWS 13	Jul 22	USAN to be reloaded July 28, 2002; saved answer sets no longer valid
NEWS 14	Jul 29	Enhanced polymer searching in REGISTRY
NEWS 15	Jul 30	NETFIRST to be removed from STN
NEWS 16	Aug 08	CANCERLIT reload
NEWS 17	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 18	Aug 08	NTIS has been reloaded and enhanced
NEWS 19	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
NEWS 20	Aug 19	IFIPAT, IFICDB, and IFIUDB have been reloaded
NEWS 21	Aug 19	The MEDLINE file segment of TOXCENTER has been reloaded
NEWS 22	Aug 26	Sequence searching in REGISTRY enhanced
NEWS 23	Sep 03	JAPIO has been reloaded and enhanced
NEWS 24	Sep 16	Experimental properties added to the REGISTRY file
NEWS 25	Sep 16	CA Section Thesaurus available in CAPLUS and CA
NEWS 26	Oct 01	CASREACT Enriched with Reactions from 1907 to 1985
NEWS 27	Oct 21	EVENTLINE has been reloaded
NEWS 28	Oct 24	BEILSTEIN adds new search fields
NEWS 29	Oct 24	Nutraceuticals International (NUTRACEUT) now available on STN
NEWS 30	Oct 25	MEDLINE SDI run of October 8, 2002
NEWS 31	Nov 18	DKILIT has been renamed APOLLIT
NEWS 32	Nov 25	More calculated properties added to REGISTRY
NEWS 33	Dec 02	TIBKAT will be removed from STN
NEWS 34	Dec 04	CSA files on STN
NEWS 35	Dec 17	PCTFULL now covers WP/PCT Applications from 1978 to date
NEWS 36	Dec 17	TOXCENTER enhanced with additional content
NEWS 37	Dec 17	Adis Clinical Trials Insight now available on STN
NEWS 38	Dec 30	ISMEC no longer available
NEWS 39	Jan 13	Indexing added to some pre-1967 records in CA/CAPLUS
NEWS 40	Jan 21	NUTRACEUT offering one free connect hour in February 2003
NEWS 41	Jan 21	PHARMAML offering one free connect hour in February 2003
NEWS 42	Jan 29	Simultaneous left and right truncation added to COMPENDEX, ENERGY, INSPEC
NEWS 43	Feb 13	CANCERLIT is no longer being updated
NEWS 44	Feb 24	METADEX enhancements
NEWS 45	Feb 24	PCTGEN now available on STN
NEWS 46	Feb 24	TEMA now available on STN

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NEWS 47  Feb 26  NTIS now allows simultaneous left and right truncation
NEWS 48  Feb 26  PCTFULL now contains images
NEWS 49  Mar 04  SDI PACKAGE for monthly delivery of multifile SDI results

NEWS EXPRESS  January 6 CURRENT WINDOWS VERSION IS V6.01a,
              CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
              AND CURRENT DISCOVER FILE IS DATED 01 OCTOBER 2002
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NEWS WWW      CAS World Wide Web Site (general information)

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=> file reg
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DICTIONARY FILE UPDATES:  16 MAR 2003  HIGHEST RN 499182-00-2

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

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Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end
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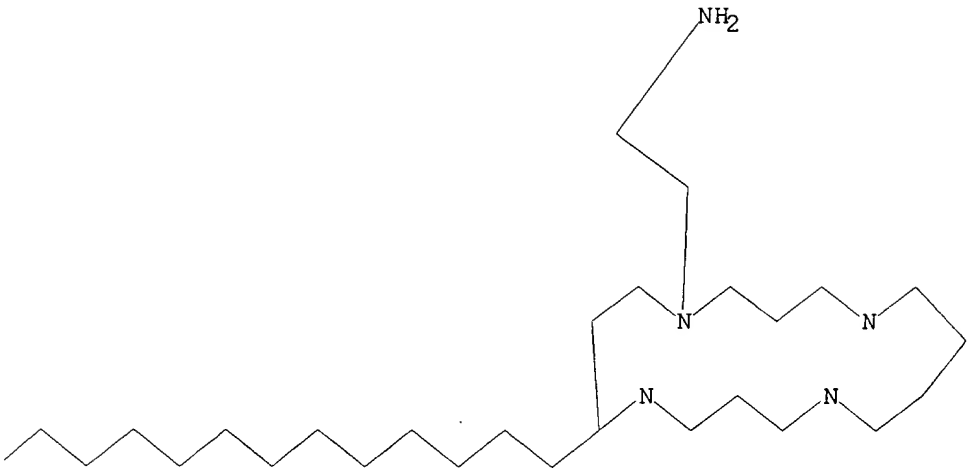
=>
Uploading C:\STNEXP4\QUERIES\922407.str

L1 STRUCTURE UPLOADED

=> que L1

L2 QUE L1

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 0 TO 0
PROJECTED ANSWERS: 0 TO 0

L3 0 SEA EXA SAM L1

=> s l1 fam sam
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SAMPLE SCREEN SEARCH COMPLETED - 8 TO ITERATE

100.0% PROCESSED 8 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 8 TO 329
PROJECTED ANSWERS: 0 TO 0

L4 0 SEA FAM SAM L1

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SAMPLE SCREEN SEARCH COMPLETED -     26 TO ITERATE

100.0% PROCESSED      26 ITERATIONS                                  0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          215 TO      825
PROJECTED ANSWERS:               0 TO        0

L5            0 SEA SSS SAM L1

=> s budmunchlamine
L6            0 BUDMUNCHLAMINE

=> s budmunchlamine
L7            0 BUDMUNCHLAMINE

=> s budmunchiamine
L8           22 BUDMUNCHIAMINE

=> d l8 1 20 22

L8   ANSWER 1 OF 22  REGISTRY  COPYRIGHT 2003 ACS
RN   195734-30-6  REGISTRY
CN   1,5,9,13-Tetraazacycloheptadecan-6-one, 8-(11-pentadecenyl)-, (+)- (9CI)
     (CA INDEX NAME)
OTHER NAMES:
CN   (+)-Budmunchiamine L6
CN   Budmunchiamine L 6
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LC   STN Files:   CA, CAPLUS

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Currently available stereo shown.
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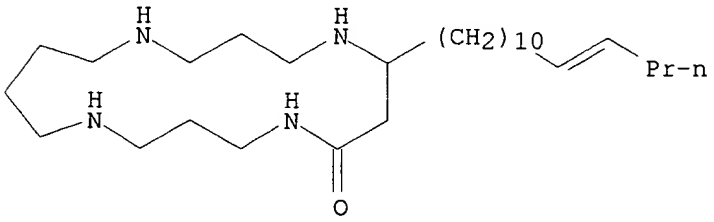


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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

             1 REFERENCES IN FILE CA (1962 TO DATE)
             1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L8   ANSWER 20 OF 22  REGISTRY  COPYRIGHT 2003 ACS
RN   139750-78-0  REGISTRY
CN   1,5,9,13-Tetraazacycloheptadecan-6-one, 1,9,13-trimethyl-8-tridecyl- (9CI)
     (CA INDEX NAME)
OTHER NAMES:
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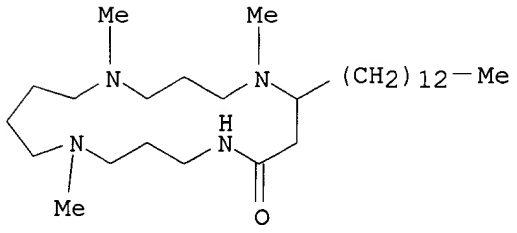
CN **Budmunchiamine C**
MF C29 H60 N4 O
SR CA
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAPLUS, CASREACT, TOXCENTER
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1962 TO DATE)
4 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L8 ANSWER 22 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 139750-76-8 REGISTRY
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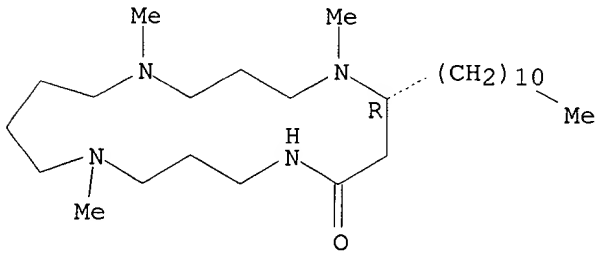
OTHER NAMES:
CN **(-)-(R)-Budmunchiamine A**
CN **Budmunchiamine A**
FS STEREOSEARCH
MF C27 H56 N4 O
SR CA
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

10 REFERENCES IN FILE CA (1962 TO DATE)
10 REFERENCES IN FILE CAPLUS (1962 TO DATE)

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FILE 'REGISTRY' ENTERED AT 13:38:20 ON 17 MAR 2003

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L1              STRUCTURE UPLOADED
L2              QUE L1
L3            0 S L1 EXA SAM
L4            0 S L1 FAM SAM
L5            0 S L1 SSS SAM
L6            0 S BUDMUNCHLAMINE
L7            0 S BUDMUNCHLAMINE
L8           22 S BUDMUNCHIAMINE

=> d l8 2-20 21

L8   ANSWER 2 OF 22  REGISTRY  COPYRIGHT 2003 ACS
RN   195734-29-3  REGISTRY
CN   1,5,9,13-Tetraazacycloheptadecan-6-one, 8-(13-heptadecenyl)-, (+)- (9CI)
     (CA INDEX NAME)
OTHER NAMES:
CN   (+)-Budmunchiamine L5
CN   Budmunchiamine L 5
FS   STEREOSEARCH
MF   C30 H60 N4 O
SR   CA
LC   STN Files:   BIOSIS, CA, CAPLUS

Rotation (+).
Double bond geometry unknown.
Currently available stereo shown.
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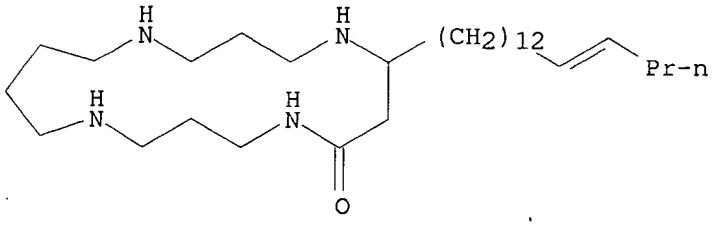


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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

              1 REFERENCES IN FILE CA (1962 TO DATE)
              1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L8   ANSWER 3 OF 22  REGISTRY  COPYRIGHT 2003 ACS
RN   195734-28-2  REGISTRY
CN   1,5,9,13-Tetraazacycloheptadecan-6-one, 8-(13-hydroxyhexadecyl)-, (+)-
     (9CI)  (CA INDEX NAME)
OTHER NAMES:
CN   (+)-Budmunchiamine L4
CN   Budmunchiamine L 4
FS   STEREOSEARCH
MF   C29 H60 N4 O2
SR   CA
LC   STN Files:   BIOSIS, CA, CAPLUS

Rotation (+).
Currently available stereo shown.
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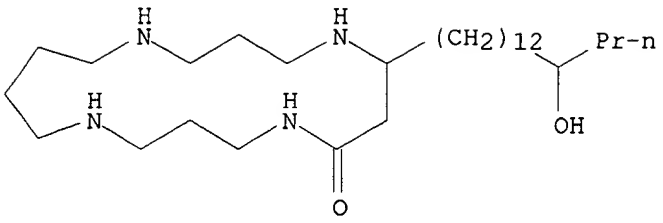
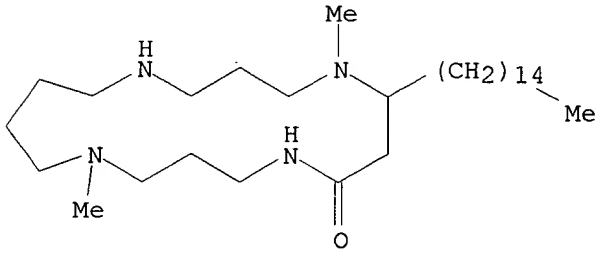


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L8 ANSWER 4 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 180285-78-3 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 1,9-dimethyl-8-pentadecyl-, (-)-
(9CI) (CA INDEX NAME)
OTHER NAMES:
CN **9-Normethylbudmunchiamine K**
FS STEREOSEARCH
MF C30 H62 N4 O
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Rotation (-).
Currently available stereo shown.

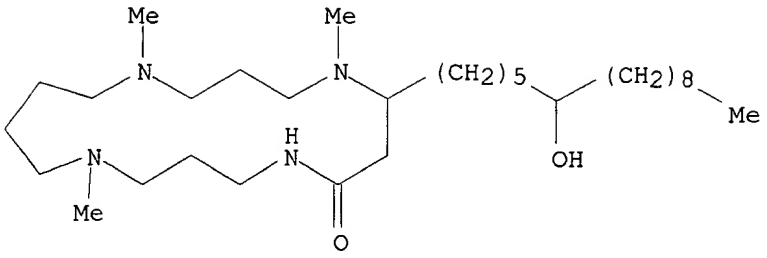


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L8 ANSWER 5 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 180285-72-7 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 8-(6-hydroxypentadecyl)-1,9,13-
trimethyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **6'.xi.-Hydroxybudmunchiamine K**
FS STEREOSEARCH
MF C31 H64 N4 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Rotation (-).
Currently available stereo shown.

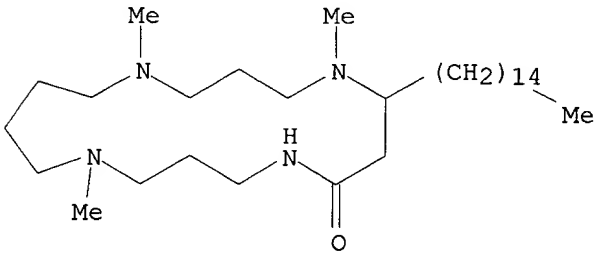


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L8 ANSWER 6 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 178494-87-6 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 1,9,13-trimethyl-8-pentadecyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine K**
MF C31 H64 N4 O
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Currently available stereo shown.

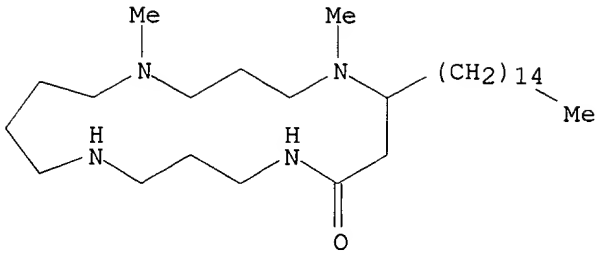


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L8 ANSWER 7 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 178494-86-5 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 9,13-dimethyl-8-pentadecyl-, (-)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **14-Normethylbudmunchiamine K**
FS STEREOSEARCH
MF C30 H62 N4 O
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Rotation (-).
Currently available stereo shown.

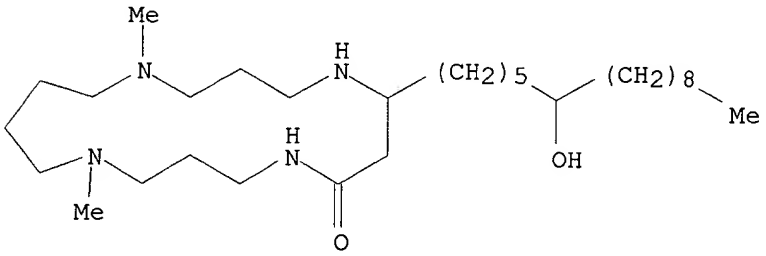


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L8 ANSWER 8 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 178494-85-4 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 8-(6-hydroxypentadecyl)-1,13-dimethyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **6'.xi.-Hydroxy-5-normethylbudmunchiamine K**
MF C30 H62 N4 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Currently available stereo shown.

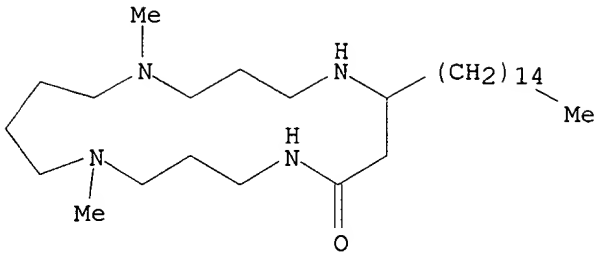


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L8 ANSWER 9 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 178494-84-3 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 1,13-dimethyl-8-pentadecyl-, (-)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **5-Normethylbudmunchiamine K**
FS STEREOSEARCH
MF C30 H62 N4 O
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Rotation (-).
Currently available stereo shown.

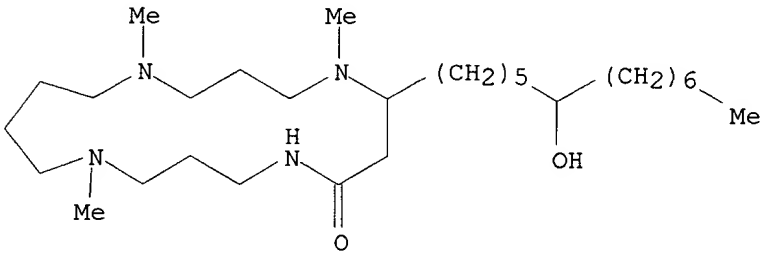


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L8 ANSWER 10 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 178494-83-2 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 8-(6-hydroxytridecyl)-1,9,13-trimethyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **6'.xi.-Hydroxybudmunchiamine C**
MF C29 H60 N4 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

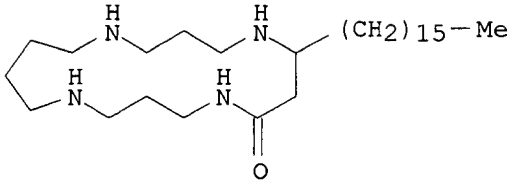
Currently available stereo shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

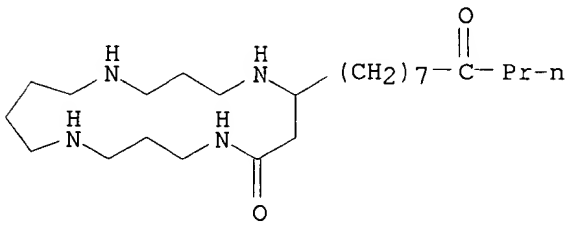
L8 ANSWER 11 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 165561-01-3 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 8-hexadecyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine L 1**
MF C29 H60 N4 O
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

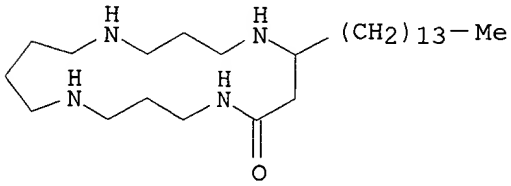
L8 ANSWER 12 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 165467-48-1 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 8-(8-oxoundecyl)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine L 3**
MF C24 H48 N4 O2
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

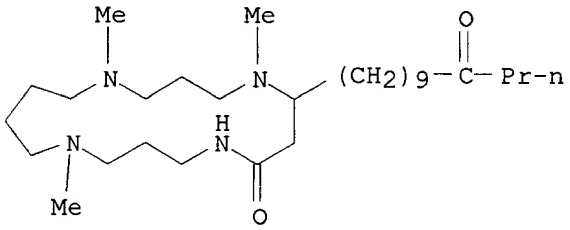
L8 ANSWER 13 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 165467-47-0 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 8-tetradecyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine L 2**
MF C27 H56 N4 O
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

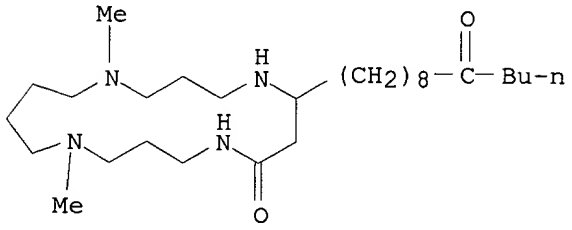
L8 ANSWER 14 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 143070-37-5 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 1,9,13-trimethyl-8-(10-oxotridecyl)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine D**
MF C29 H58 N4 O2
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

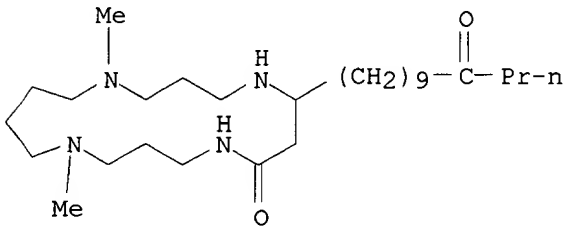
L8 ANSWER 15 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 143051-90-5 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 1,13-dimethyl-8-(9-oxotridecyl)-(9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine I**
MF C28 H56 N4 O2
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

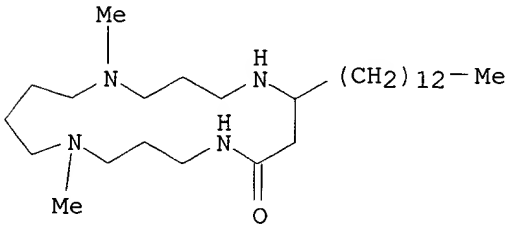
L8 ANSWER 16 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 143051-89-2 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 1,13-dimethyl-8-(10-oxododecyl)-
(9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine H**
MF C28 H56 N4 O2
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L8 ANSWER 17 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 143051-88-1 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 1,13-dimethyl-8-tridecyl- (9CI)
(CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine G**
MF C28 H58 N4 O
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

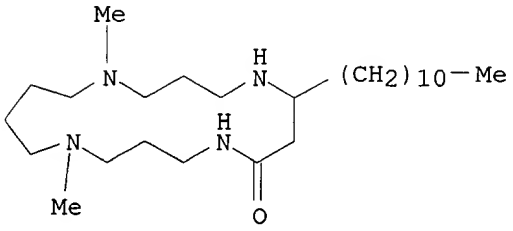


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L8 ANSWER 18 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 143051-87-0 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 1,13-dimethyl-8-undecyl- (9CI)
(CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine F**

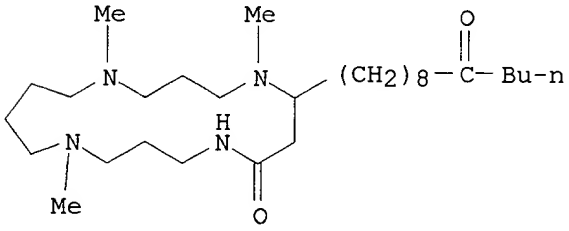
MF C26 H54 N4 O
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

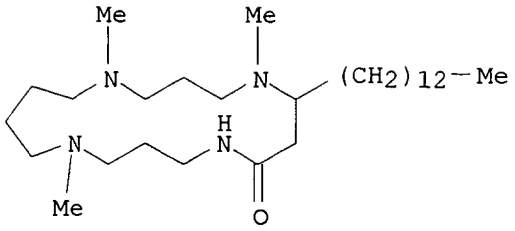
L8 ANSWER 19 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 143051-86-9 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 1,9,13-trimethyl-8-(9-oxotridecyl)-(9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine E**
MF C29 H58 N4 O2
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

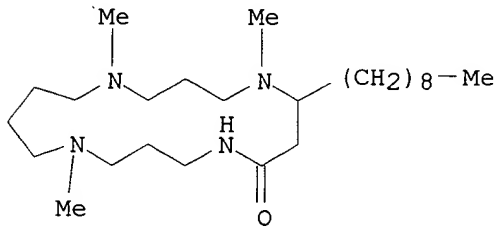
L8 ANSWER 20 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 139750-78-0 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 1,9,13-trimethyl-8-tridecyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine C**
MF C29 H60 N4 O
SR CA
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAPLUS, CASREACT, TOXCENTER
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1962 TO DATE)
4 REFERENCES IN FILE CAPLUS (1962 TO DATE)

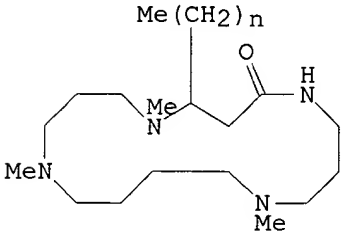
L8 ANSWER 21 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 139750-77-9 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 1,9,13-trimethyl-8-nonyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine B**
MF C25 H52 N4 O
SR CA
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAPLUS, CASREACT, TOXCENTER
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1962 TO DATE)
4 REFERENCES IN FILE CAPLUS (1962 TO DATE)

AN 117:23236 CA
TI DNA-based isolation and the structure elucidation of the budmunchiamines, novel macrocyclic alkaloids from Albizia amara
AU Pezzuto, John M.; Mar, Woongchon; Lin, Long Ze; Cordell, Geoffrey A.; Neszmelyi, Andras; Wagner, Hildebert
CS Coll. Pharm., Univ. Illinois, Chicago, IL, USA
SO Heterocycles (1991), 32(10), 1961-7
CODEN: HTCYAM; ISSN: 0385-5414
DT Journal
LA English
CC 11-1 (Plant Biochemistry)
Section cross-reference(s): 31
GI



I, n=10
II, n=8
III, n=12

AB On the basis of DNA affinity, a novel isolate was obtained from an ext. prepd. from the seeds of A. amara. As detd. by a series of spectroscopic techniques, the isolate was structurally defined as a mixt. of 3 macrocyclic alkaloids of the pithecolobine type that differed only in the length of the aliph. side chain. The 1H- and 13C-NMR spectral parameters were unambiguously assigned to these alkaloids, which were given the trivial names budmunchiamine A (I), B (II), or C (III). With the exception of former studies performed with Pithecolobium saman, this is the only other reported of pithecolobine alkaloids being found in nature.
ST Albizia pithecolobine alkaloid budmunchiamine
IT Nomenclature, new natural products
(budmunchiamine A (alkaloid))
IT Nomenclature, new natural products
(budmunchiamine B (alkaloid))
IT Nomenclature, new natural products
(budmunchiamine C (alkaloid))
IT Albizia amara
(macrocyclic alkaloids from, structure of)
IT Molecular structure, natural product
(of budmunchiamine A (alkaloid))
IT Molecular structure, natural product
(of budmunchiamine B (alkaloid))
IT Molecular structure, natural product
(of budmunchiamine C (alkaloid))
IT Alkaloids, biological studies
RL: BIOL (Biological study)
(macrocyclic, pithecolobine, from Albizia amara)
IT 139750-76-8, Budmunchiamine A 139750-77-9, Budmunchiamine B 139750-78-0, Budmunchiamine C
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of Albizia amara, isolation and structure detn. of)

Welcome to STN International! Enter x:x

LOGINID:sssptau125rxt

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2	Apr 08	"Ask CAS" for self-help around the clock
NEWS 3	Apr 09	BEILSTEIN: Reload and Implementation of a New Subject Area
NEWS 4	Apr 09	ZDB will be removed from STN
NEWS 5	Apr 19	US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
NEWS 6	Apr 22	Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
NEWS 7	Apr 22	BIOSIS Gene Names now available in TOXCENTER
NEWS 8	Apr 22	Federal Research in Progress (FEDRIP) now available
NEWS 9	Jun 03	New e-mail delivery for search results now available
NEWS 10	Jun 10	MEDLINE Reload
NEWS 11	Jun 10	PCTFULL has been reloaded
NEWS 12	Jul 02	FOREGE no longer contains STANDARDS file segment
NEWS 13	Jul 22	USAN to be reloaded July 28, 2002; saved answer sets no longer valid
NEWS 14	Jul 29	Enhanced polymer searching in REGISTRY
NEWS 15	Jul 30	NETFIRST to be removed from STN
NEWS 16	Aug 08	CANCERLIT reload
NEWS 17	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 18	Aug 08	NTIS has been reloaded and enhanced
NEWS 19	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
NEWS 20	Aug 19	IFIPAT, IFICDB, and IFIUDB have been reloaded
NEWS 21	Aug 19	The MEDLINE file segment of TOXCENTER has been reloaded
NEWS 22	Aug 26	Sequence searching in REGISTRY enhanced
NEWS 23	Sep 03	JAPIO has been reloaded and enhanced
NEWS 24	Sep 16	Experimental properties added to the REGISTRY file
NEWS 25	Sep 16	CA Section Thesaurus available in CAPLUS and CA
NEWS 26	Oct 01	CASREACT Enriched with Reactions from 1907 to 1985
NEWS 27	Oct 21	EVENTLINE has been reloaded
NEWS 28	Oct 24	BEILSTEIN adds new search fields
NEWS 29	Oct 24	Nutraceuticals International (NUTRACEUT) now available on STN
NEWS 30	Oct 25	MEDLINE SDI run of October 8, 2002
NEWS 31	Nov 18	DKILIT has been renamed APOLLIT
NEWS 32	Nov 25	More calculated properties added to REGISTRY
NEWS 33	Dec 02	TIBKAT will be removed from STN
NEWS 34	Dec 04	CSA files on STN
NEWS 35	Dec 17	PCTFULL now covers WP/PCT Applications from 1978 to date
NEWS 36	Dec 17	TOXCENTER enhanced with additional content
NEWS 37	Dec 17	Adis Clinical Trials Insight now available on STN
NEWS 38	Dec 30	ISMEC no longer available
NEWS 39	Jan 13	Indexing added to some pre-1967 records in CA/CAPLUS
NEWS 40	Jan 21	NUTRACEUT offering one free connect hour in February 2003
NEWS 41	Jan 21	PHARMAML offering one free connect hour in February 2003
NEWS 42	Jan 29	Simultaneous left and right truncation added to COMPENDEX, ENERGY, INSPEC
NEWS 43	Feb 13	CANCERLIT is no longer being updated
NEWS 44	Feb 24	METADEX enhancements
NEWS 45	Feb 24	PCTGEN now available on STN
NEWS 46	Feb 24	TEMA now available on STN

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NEWS 47  Feb 26  NTIS now allows simultaneous left and right truncation
NEWS 48  Feb 26  PCTFULL now contains images
NEWS 49  Mar 04  SDI PACKAGE for monthly delivery of multifile SDI results

NEWS EXPRESS  January 6 CURRENT WINDOWS VERSION IS V6.01a,
              CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
              AND CURRENT DISCOVER FILE IS DATED 01 OCTOBER 2002
NEWS HOURS    STN Operating Hours Plus Help Desk Availability
NEWS INTER    General Internet Information
NEWS LOGIN    Welcome Banner and News Items
NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
NEWS WWW      CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
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  * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *



FILE 'HOME' ENTERED AT 12:58:18 ON 18 MAR 2003

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.21       0.21

FILE 'REGISTRY' ENTERED AT 12:58:26 ON 18 MAR 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   17 MAR 2003  HIGHEST RN 499763-93-8
DICTIONARY FILE UPDATES:  17 MAR 2003  HIGHEST RN 499763-93-8

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end
```

=>
Uploading C:\STNEXP4\QUERIES\922407b.str

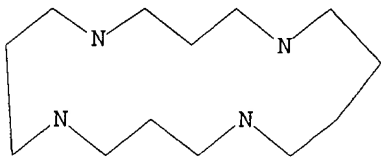
L1 STRUCTURE UPLOADED

=> que L1

L2 QUE L1

=> id l1
ID IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 exa sam
SAMPLE SEARCH INITIATED 12:59:17 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1 TO 80
PROJECTED ANSWERS: 0 TO 0

L3 0 SEA EXA SAM L1

=> s l1 fam sam
SAMPLE SEARCH INITIATED 12:59:27 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1080 TO ITERATE

92.6% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 19629 TO 23571
PROJECTED ANSWERS: 0 TO 0

L4 0 SEA FAM SAM L1

=> s l1 sss sam
SAMPLE SEARCH INITIATED 12:59:40 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 5730 TO ITERATE

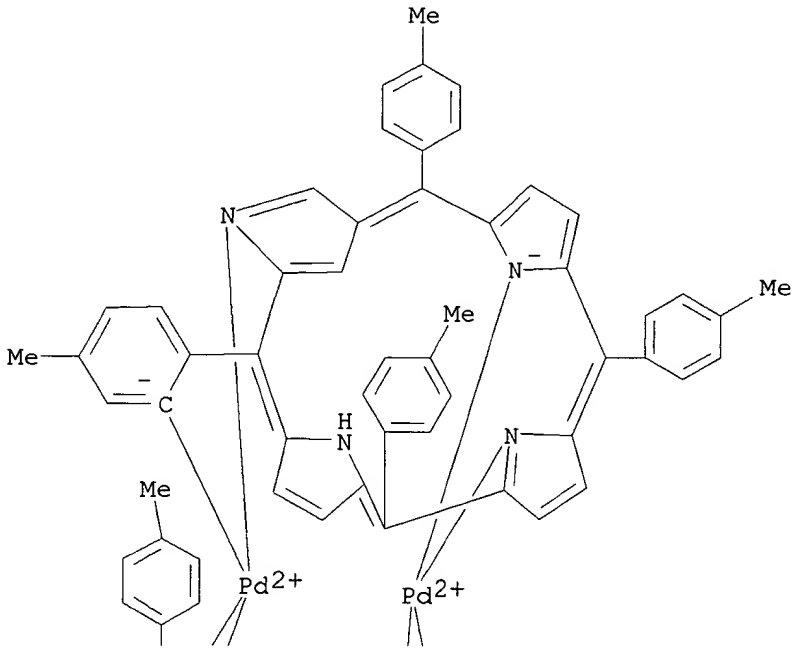
17.5% PROCESSED 1000 ITERATIONS 2 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

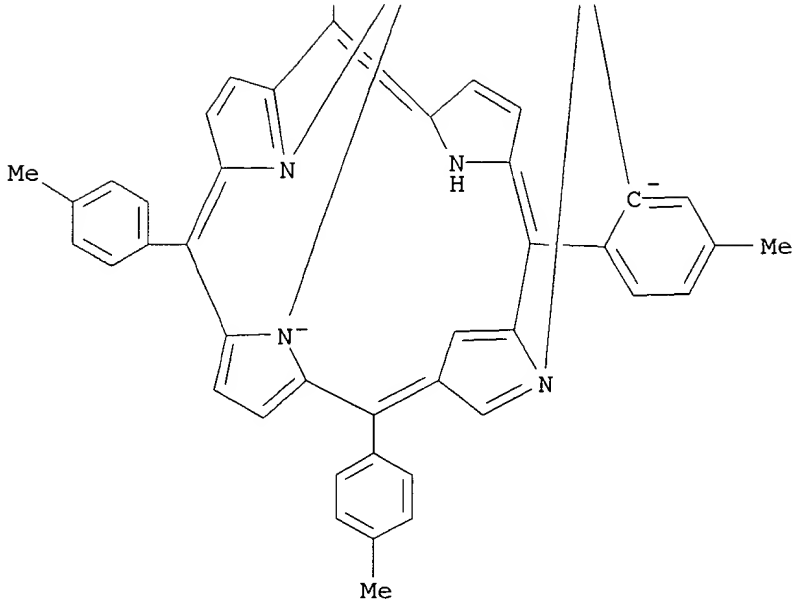
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 110064 TO 119136
PROJECTED ANSWERS: 26 TO 432

L5 2 SEA SSS SAM L1

=> d l5 1-2

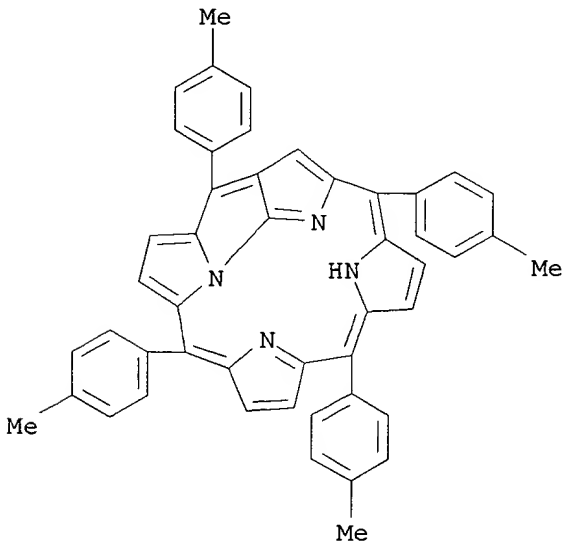
L5 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2003 ACS
RN 316384-92-6 REGISTRY
CN Palladium, bis[.mu.-[2-(4-methylphenyl-.kappa.C2)-7,12,17-tris(4-methylphenyl)-4,21,22,23-tetraazapentacyclo[16.2.1.13,6.18,11.113,16]tetracosa-1,3(24),4,6,8,10,12,14,16(22),17,19-undecaenato(2-)-.kappa.N4:.kappa.N22,.kappa.N23]]di- (9CI) (CA INDEX NAME)
MF C96 H72 N8 Pd2
CI CCS
SR CA
LC STN Files: CA, CAPLUS





1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L5 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2003 ACS
RN 289659-14-9 REGISTRY
CN 4,7-Imino-17,2-metheno-12,9-nitrilo[1,3]diazacyclohexadecino[2,1,16-cd]pyrrolizine, 3,8,13,16-tetrakis(4-methylphenyl)- (9CI) (CA INDEX NAME)
MF C48 H36 N4
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

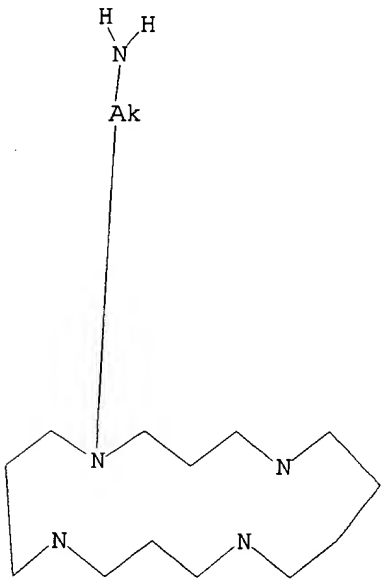
=>
Uploading C:\STNEXP4\QUERIES\922407a.str

L6 STRUCTURE UPLOADED

=> que L6

L7 QUE L6

=> d l6
L6 HAS NO ANSWERS
L6 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l6 sss full
FULL SEARCH INITIATED 13:01:53 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 113635 TO ITERATE

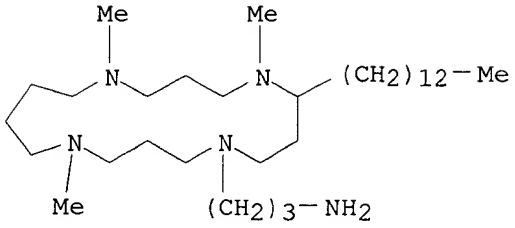
100.0% PROCESSED 113635 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.05

L8 2 SEA SSS FUL L6

=> d l8 1-2

L8 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2003 ACS
RN 396117-44-5 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecane-5-propanamine, 1,9,13-trimethyl-8-tridecyl-, pentahydrochloride (9CI) (CA INDEX NAME)
OTHER NAMES:
CN SL 11239

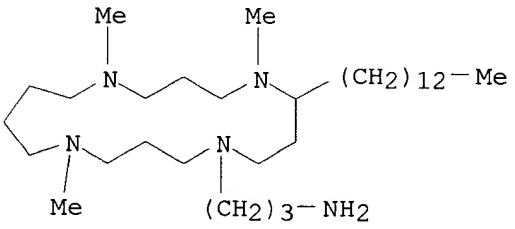
MF C32 H69 N5 . 5 Cl H
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
CRN (395649-55-5)



●5 HCl

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L8 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2003 ACS
RN 395649-55-5 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecane-5-propanamine, 1,9,13-trimethyl-8-tridecyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C32 H69 N5
CI COM
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

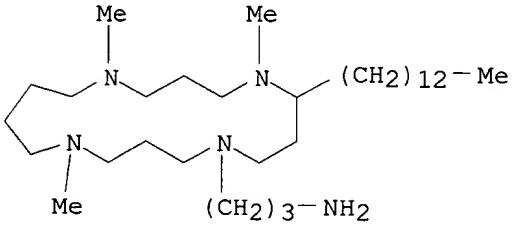
=> d l8 1 all

L8 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2003 ACS
RN 396117-44-5 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecane-5-propanamine, 1,9,13-trimethyl-8-tridecyl-, pentahydrochloride (9CI) (CA INDEX NAME)
OTHER NAMES:
CN SL 11239
MF C32 H69 N5 . 5 Cl H
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

CRN (395649-55-5)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C13N4	NC3NC3NC3NC4	17	C13N4	4584.21.1	1



●5 HCl

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

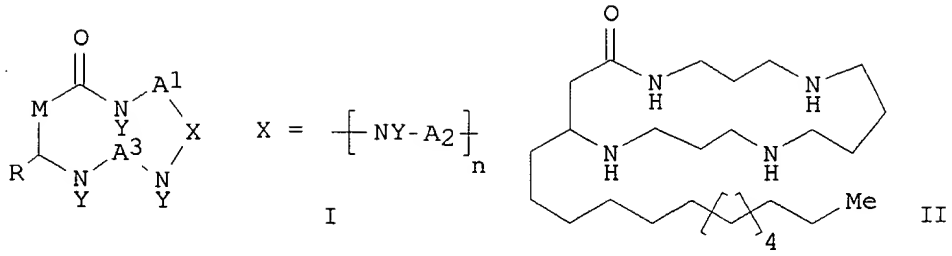
REFERENCE 1

AN 136:167548 CA
TI Synthesis of cyclic polyamine analogs for cancer therapy
IN Frydman, Benjamin; Hesse, Manfred; Guggisberg, Armin; Popaj, Kasmin; Drandarov, Konstantin; Basu, Hirak; Bhattacharya, Subhra; Wang, Yu
PA Slil Biomedical Corporation, USA
SO PCT Int. Appl., 105 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D257-02
ICS C07D255-02; A61K031-395; A61P035-00
CC 31-6 (Alkaloids)
Section cross-reference(s): 1
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002010142	A1	20020207	WO 2001-US24282	20010802

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2000-222522P 20000802
GI



I II

AB Novel cyclic polyamine compds., such as I [A1, A2 = C1-C8 alkyl; Y = H, C1-C4 alkyl; M = C1-C4 alkyl; n = 0-3; R = C1-C32 alkyl], as well as all stereoisomers and salts thereof, were prepd. for treating diseases caused by uncontrolled proliferation of cells, such as cancer, esp. prostate cancer, and for inducing intracellular ATP hydrolysis for treatment of other disorders. Thus, cyclic polyamine II was prepd. via multistep synthetic sequence starting from triphenylphosphine, Et bromoacetate, myristylaldehyde and spermine. II.3HCl showed ID50 = 0.83.mu.M on prostate tumor cell growth.

ST polyamine cyclic prepn anticancer budmunchiamine

IT Polyamines
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(analog; prepn. of cyclic polyamine analogs for cancer therapy)

IT Cyclization
(lactamization, macrolactamization; in prepn. of cyclic polyamine analogs for cancer therapy)

IT Macrocyclization
(macrolactamization; in prepn. of cyclic polyamine analogs for cancer therapy)

IT Prostate gland
(neoplasm, inhibitors; prepn. of cyclic polyamine analogs for cancer therapy)

IT Cytotoxicity
(of cyclic polyamine analogs on survival of DuPro cells)

IT Alkylation
(of secondary amino groups in prepn. of cyclic polyamine analogs for cancer therapy)

IT Peptides, biological studies
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pentapeptides; prepn. of cyclic polyamine analogs for cancer therapy)

IT Antitumor agents
(prostate gland; prepn. of cyclic polyamine analogs for cancer therapy)

IT Peptides, biological studies
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(tetrapeptides; prepn. of cyclic polyamine analogs for cancer therapy)

IT 56-65-5, ATP, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(hydrolysis; in a cancerous cell via cyclic polyamine analogs)

IT 4375-83-1, Tris(dimethylamino)borane
RL: RGT (Reagent); RACT (Reactant or reagent)
(in prepn. of cyclic polyamine analogs for cancer therapy)

IT 139750-76-8P 139750-77-9P 396117-44-5P, SL 11239 396117-45-6P, SL 11238 396117-46-7P, SL 11174 396117-47-8P, SL 11197 396117-48-9P, SL 11199 396117-49-0P, SL 11200 396117-50-3P, SL 11208
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

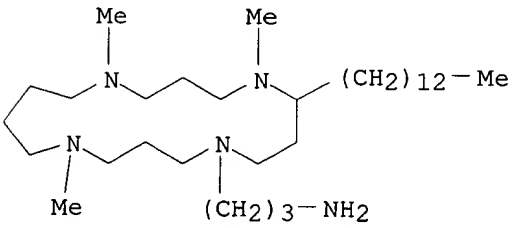
(prepn. of cyclic polyamine analogs for cancer therapy)
IT 395649-52-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of cyclic polyamine analogs for cancer therapy)
IT 110-60-1P, Putrescine 124-20-9P, Spermidine
RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of cyclic polyamine analogs for cancer therapy)
IT 50-00-0, Formalin, reactions 71-44-3, Spermine 105-36-2, Ethyl bromoacetate 107-13-1, Acrylonitrile, reactions 112-31-2, Caprinaldehyde 112-54-9, Laurinaldehyde 124-25-4, Myristinaldehyde 603-35-0, Triphenylphosphine, reactions 73453-98-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of cyclic polyamine analogs for cancer therapy)
IT 1530-45-6P 28290-90-6P 38112-60-6P 42778-95-0P 75814-58-3P 135251-95-5P 139750-78-0P, Budmunchiamine C 335153-35-0P 335153-39-4P 335153-41-8P 335153-43-0P 395649-49-7P 395649-50-0P 395649-51-1P 395649-53-3P 395649-54-4P 395649-55-5P 395649-56-6P 395649-57-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of cyclic polyamine analogs for cancer therapy)
IT 10433-06-4, Antimony(III)ethoxide 25895-60-7, Sodium cyanoborohydride
RL: RGT (Reagent); RACT (Reactant or reagent)
(prepn. of cyclic polyamine analogs for cancer therapy)
RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Squibb Bristol Myers Co; EP 0451547 A 1991 CAPLUS
(2) Univ Hawaii; EP 0792875 A 1997 CAPLUS

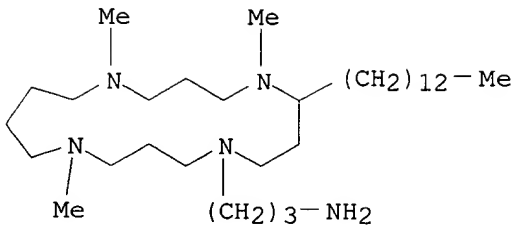
=> d l8 2 all

L8 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2003 ACS
RN 395649-55-5 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecane-5-propanamine, 1,9,13-trimethyl-8-tridecyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C32 H69 N5
CI COM
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C13N4	NC3NC3NC3NC4	17	C13N4	4584.21.1	1





Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1	pH 1	(1) ACD
Bioconc. Factor (BCF)	1	pH 4	(1) ACD
Bioconc. Factor (BCF)	1	pH 7	(1) ACD
Bioconc. Factor (BCF)	3.78	pH 8	(1) ACD
Bioconc. Factor (BCF)	419479	pH 10	(1) ACD
Boiling Point (BP)	595.8+/-50.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	88.78+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	308.7+/-44.8 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	16		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	2		(1) ACD
Koc (KOC)	1	pH 1	(1) ACD
Koc (KOC)	1	pH 4	(1) ACD
Koc (KOC)	1	pH 7	(1) ACD
Koc (KOC)	1.81	pH 8	(1) ACD
Koc (KOC)	200599	pH 10	(1) ACD
logD (LOGD)	0.92	pH 1	(1) ACD
logD (LOGD)	0.93	pH 4	(1) ACD
logD (LOGD)	1.86	pH 7	(1) ACD
logD (LOGD)	2.95	pH 8	(1) ACD
logD (LOGD)	7.99	pH 10	(1) ACD
logP (LOGP)	8.923+/-0.454		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	523.92		(1) ACD
pKa (PKA)	10.45+/-0.10	Most Basic	(1) ACD
Vapor Pressure (VP)	3.67E-14 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD)

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1

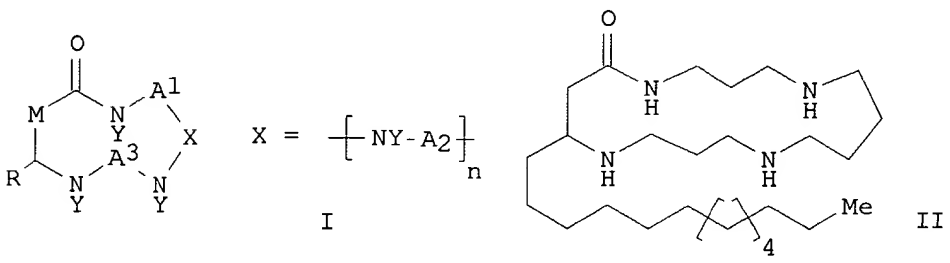
AN 136:167548 CA
TI Synthesis of cyclic polyamine analogs for cancer therapy
IN Frydman, Benjamin; Hesse, Manfred; Guggisberg, Armin; Popaj, Kasmin; Drandarov, Konstantin; Basu, Hirak; Bhattacharya, Subhra; Wang, Yu
PA Slil Biomedical Corporation, USA

SO PCT Int. Appl., 105 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D257-02
ICS C07D255-02; A61K031-395; A61P035-00
CC 31-6 (Alkaloids)
Section cross-reference(s): 1
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002010142	A1	20020207	WO 2001-US24282	20010802

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2000-222522P 20000802
GI



AB Novel cyclic polyamine compds., such as I [A1, A2 = C1-C8 alkyl; Y = H, C1-C4 alkyl; M = C1-C4 alkyl; n = 0-3; R = C1-C32 alkyl], as well as all stereoisomers and salts thereof, were prepd. for treating diseases caused by uncontrolled proliferation of cells, such as cancer, esp. prostate cancer, and for inducing intracellular ATP hydrolysis for treatment of other disorders. Thus, cyclic polyamine II was prepd. via multistep synthetic sequence starting from triphenylphosphine, Et bromoacetate, myristylaldehyde and spermine. II.3HCl showed ID50 = 0.83.mu.M on prostate tumor cell growth.
ST polyamine cyclic prepn anticancer budmunchiamine
IT Polyamines
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(analog; prepn. of cyclic polyamine analogs for cancer therapy)
IT Cyclization
(lactamization, macrolactamization; in prepn. of cyclic polyamine analogs for cancer therapy)
IT Macrocyclization
(macrolactamization; in prepn. of cyclic polyamine analogs for cancer therapy)
IT Prostate gland
(neoplasm, inhibitors; prepn. of cyclic polyamine analogs for cancer therapy)
IT Cytotoxicity

(of cyclic polyamine analogs on survival of DuPro cells)
IT Alkylation
(of secondary amino groups in prepn. of cyclic polyamine analogs for cancer therapy)
IT Peptides, biological studies
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pentapeptides; prepn. of cyclic polyamine analogs for cancer therapy)
IT Antitumor agents
(prostate gland; prepn. of cyclic polyamine analogs for cancer therapy)
IT Peptides, biological studies
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(tetrapeptides; prepn. of cyclic polyamine analogs for cancer therapy)
IT 56-65-5, ATP, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(hydrolysis; in a cancerous cell via cyclic polyamine analogs)
IT 4375-83-1, Tris(dimethylamino)borane
RL: RGT (Reagent); RACT (Reactant or reagent)
(in prepn. of cyclic polyamine analogs for cancer therapy)
IT 139750-76-8P 139750-77-9P 396117-44-5P, SL 11239 396117-45-6P, SL 11238 396117-46-7P, SL 11174 396117-47-8P, SL 11197 396117-48-9P, SL 11199 396117-49-0P, SL 11200 396117-50-3P, SL 11208
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of cyclic polyamine analogs for cancer therapy)
IT 395649-52-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of cyclic polyamine analogs for cancer therapy)
IT 110-60-1P, Putrescine 124-20-9P, Spermidine
RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of cyclic polyamine analogs for cancer therapy)
IT 50-00-0, Formalin, reactions 71-44-3, Spermine 105-36-2, Ethyl bromoacetate 107-13-1, Acrylonitrile, reactions 112-31-2, Caprinaldehyde 112-54-9, Laurinaldehyde 124-25-4, Myristinaldehyde 603-35-0, Triphenylphosphine, reactions 73453-98-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of cyclic polyamine analogs for cancer therapy)
IT 1530-45-6P 28290-90-6P 38112-60-6P 42778-95-0P 75814-58-3P 135251-95-5P 139750-78-0P, Budmunchiamine C 335153-35-0P 335153-39-4P 335153-41-8P 335153-43-0P 395649-49-7P 395649-50-0P 395649-51-1P 395649-53-3P 395649-54-4P 395649-55-5P 395649-56-6P 395649-57-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of cyclic polyamine analogs for cancer therapy)
IT 10433-06-4, Antimony(III)ethoxide 25895-60-7, Sodium cyanoborohydride
RL: RGT (Reagent); RACT (Reactant or reagent)
(prepn. of cyclic polyamine analogs for cancer therapy)
RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Squibb Bristol Myers Co; EP 0451547 A 1991 CAPLUS
(2) Univ Hawaii; EP 0792875 A 1997 CAPLUS

=> d his

(FILE 'HOME' ENTERED AT 12:58:18 ON 18 MAR 2003)

FILE 'REGISTRY' ENTERED AT 12:58:26 ON 18 MAR 2003
L1 STRUCTURE UPLOADED

```
L2              QUE L1
L3            0 S L1 EXA SAM
L4            0 S L1 FAM SAM
L5            2 S L1 SSS SAM
L6              STRUCTURE UPLOADED
L7              QUE L6
L8            2 S L6 SSS FULL
```

Welcome to STN International! Enter x:x

LOGINID:sssptau125rxt

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2	Apr 08	"Ask CAS" for self-help around the clock
NEWS 3	Apr 09	BEILSTEIN: Reload and Implementation of a New Subject Area
NEWS 4	Apr 09	ZDB will be removed from STN
NEWS 5	Apr 19	US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
NEWS 6	Apr 22	Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
NEWS 7	Apr 22	BIOSIS Gene Names now available in TOXCENTER
NEWS 8	Apr 22	Federal Research in Progress (FEDRIP) now available
NEWS 9	Jun 03	New e-mail delivery for search results now available
NEWS 10	Jun 10	MEDLINE Reload
NEWS 11	Jun 10	PCTFULL has been reloaded
NEWS 12	Jul 02	FOREGE no longer contains STANDARDS file segment
NEWS 13	Jul 22	USAN to be reloaded July 28, 2002; saved answer sets no longer valid
NEWS 14	Jul 29	Enhanced polymer searching in REGISTRY
NEWS 15	Jul 30	NETFIRST to be removed from STN
NEWS 16	Aug 08	CANCERLIT reload
NEWS 17	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 18	Aug 08	NTIS has been reloaded and enhanced
NEWS 19	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
NEWS 20	Aug 19	IFIPAT, IFICDB, and IFIUDB have been reloaded
NEWS 21	Aug 19	The MEDLINE file segment of TOXCENTER has been reloaded
NEWS 22	Aug 26	Sequence searching in REGISTRY enhanced
NEWS 23	Sep 03	JAPIO has been reloaded and enhanced
NEWS 24	Sep 16	Experimental properties added to the REGISTRY file
NEWS 25	Sep 16	CA Section Thesaurus available in CAPLUS and CA
NEWS 26	Oct 01	CASREACT Enriched with Reactions from 1907 to 1985
NEWS 27	Oct 21	EVENTLINE has been reloaded
NEWS 28	Oct 24	BEILSTEIN adds new search fields
NEWS 29	Oct 24	Nutraceuticals International (NUTRACEUT) now available on STN
NEWS 30	Oct 25	MEDLINE SDI run of October 8, 2002
NEWS 31	Nov 18	DKILIT has been renamed APOLLIT
NEWS 32	Nov 25	More calculated properties added to REGISTRY
NEWS 33	Dec 02	TIBKAT will be removed from STN
NEWS 34	Dec 04	CSA files on STN
NEWS 35	Dec 17	PCTFULL now covers WP/PCT Applications from 1978 to date
NEWS 36	Dec 17	TOXCENTER enhanced with additional content
NEWS 37	Dec 17	Adis Clinical Trials Insight now available on STN
NEWS 38	Dec 30	ISMEC no longer available
NEWS 39	Jan 13	Indexing added to some pre-1967 records in CA/CAPLUS
NEWS 40	Jan 21	NUTRACEUT offering one free connect hour in February 2003
NEWS 41	Jan 21	PHARMAML offering one free connect hour in February 2003
NEWS 42	Jan 29	Simultaneous left and right truncation added to COMPENDEX, ENERGY, INSPEC
NEWS 43	Feb 13	CANCERLIT is no longer being updated
NEWS 44	Feb 24	METADEX enhancements
NEWS 45	Feb 24	PCTGEN now available on STN
NEWS 46	Feb 24	TEMA now available on STN

```
 NEWS 47  Feb 26  NTIS now allows simultaneous left and right truncation
 NEWS 48  Feb 26  PCTFULL now contains images
 NEWS 49  Mar 04  SDI PACKAGE for monthly delivery of multifile SDI results

 NEWS EXPRESS  January 6 CURRENT WINDOWS VERSION IS V6.01a,
               CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
               AND CURRENT DISCOVER FILE IS DATED 01 OCTOBER 2002
 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)

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  * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * *



FILE 'HOME' ENTERED AT 12:58:18 ON 18 MAR 2003

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.21       0.21

FILE 'REGISTRY' ENTERED AT 12:58:26 ON 18 MAR 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   17 MAR 2003  HIGHEST RN 499763-93-8
DICTIONARY FILE UPDATES:  17 MAR 2003  HIGHEST RN 499763-93-8

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end
```

```
=>
Uploading C:\STNEXP4\QUERIES\922407b.str

L1      STRUCTURE UPLOADED

=> que L1

L2   QUE L1

=> id l1
ID IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> d l1
L1 HAS NO ANSWERS
L1               STR
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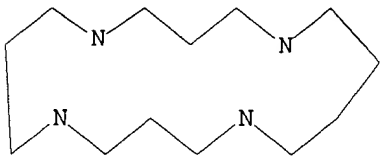


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Structure attributes must be viewed using STN Express query preparation.


=> s l1 exa sam
SAMPLE SEARCH INITIATED 12:59:17 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      1 TO ITERATE

100.0% PROCESSED       1 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            1 TO       80
PROJECTED ANSWERS:               0 TO        0

L3            0 SEA EXA SAM L1

=> s l1 fam sam
SAMPLE SEARCH INITIATED 12:59:27 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   1080 TO ITERATE

 92.6% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        19629 TO    23571
PROJECTED ANSWERS:               0 TO        0

L4            0 SEA FAM SAM L1

=> s l1 sss sam
SAMPLE SEARCH INITIATED 12:59:40 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   5730 TO ITERATE
```

17.5% PROCESSED 1000 ITERATIONS 2 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

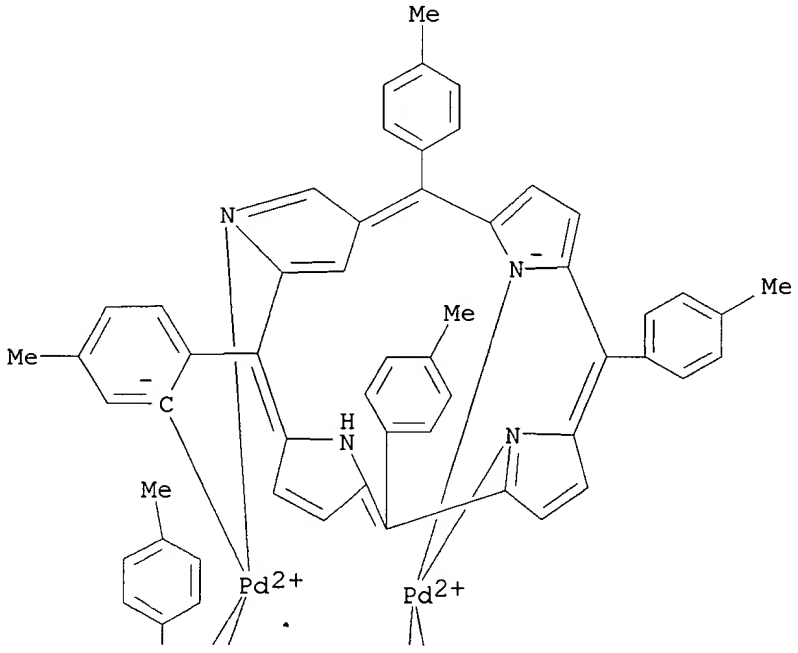
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 110064 TO 119136
PROJECTED ANSWERS: 26 TO 432

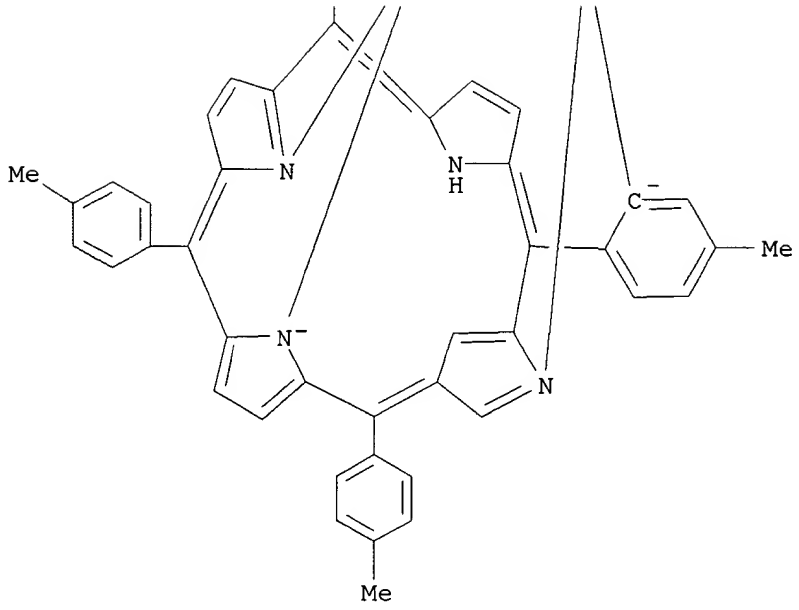
L5 2 SEA SSS SAM L1

=> d l5 1-2

L5 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2003 ACS
RN 316384-92-6 REGISTRY
CN Palladium, bis[.mu.-[2-(4-methylphenyl-.kappa.C2)-7,12,17-tris(4-methylphenyl)-4,21,22,23-tetraazapentacyclo[16.2.1.13,6.18,11.113,16]tetracosa-1,3(24),4,6,8,10,12,14,16(22),17,19-undecaenato(2-)-.kappa.N4:.kappa.N22,.kappa.N23]]di- (9CI) (CA INDEX NAME)
MF C96 H72 N8 Pd2
CI CCS
SR CA
LC STN Files: CA, CAPLUS

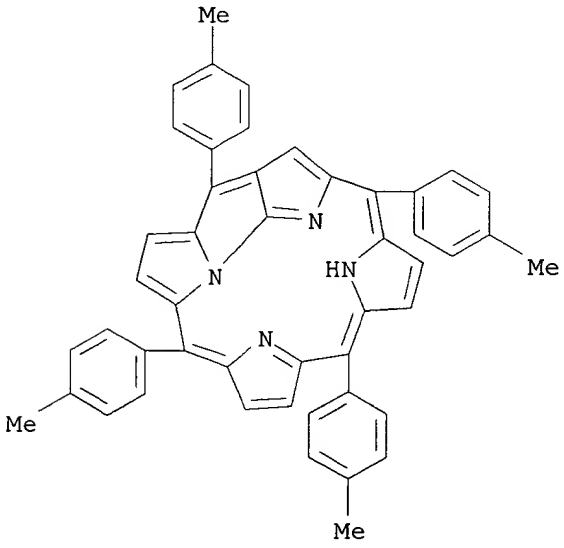
PAGE 1-A





1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L5 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2003 ACS
RN 289659-14-9 REGISTRY
CN 4,7-Imino-17,2-metheno-12,9-nitrilo[1,3]diazacyclohexadecino[2,1,16-cd]pyrrolizine, 3,8,13,16-tetrakis(4-methylphenyl)- (9CI) (CA INDEX NAME)
MF C48 H36 N4
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

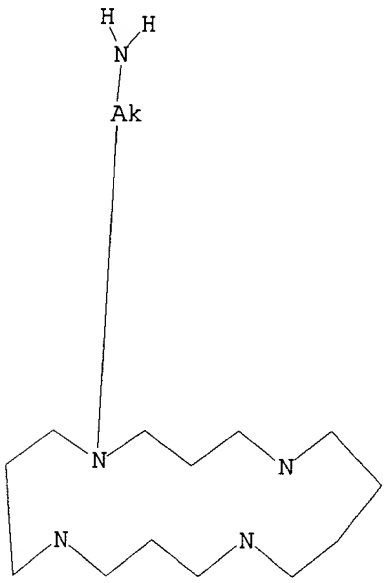
=>
Uploading C:\STNEXP4\QUERIES\922407a.str

L6 STRUCTURE UPLOADED

=> que L6

L7 QUE L6

=> d l6
L6 HAS NO ANSWERS
L6 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l6 sss full
FULL SEARCH INITIATED 13:01:53 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 113635 TO ITERATE

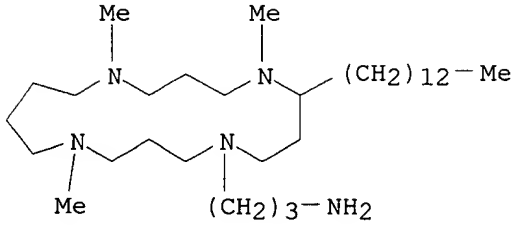
100.0% PROCESSED 113635 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.05

L8 2 SEA SSS FUL L6

=> d l8 1-2

L8 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2003 ACS
RN 396117-44-5 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecane-5-propanamine, 1,9,13-trimethyl-8-tridecyl-, pentahydrochloride (9CI) (CA INDEX NAME)
OTHER NAMES:
CN SL 11239

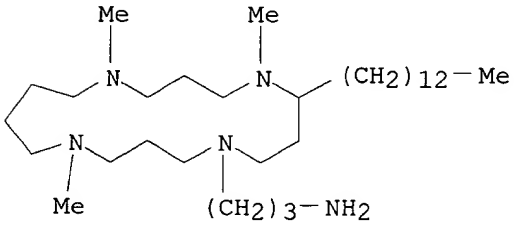
MF C32 H69 N5 . 5 Cl H
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
CRN (395649-55-5)



● 5 HCl

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L8 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2003 ACS
RN 395649-55-5 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecane-5-propanamine, 1,9,13-trimethyl-8-tridecyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C32 H69 N5
CI COM
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

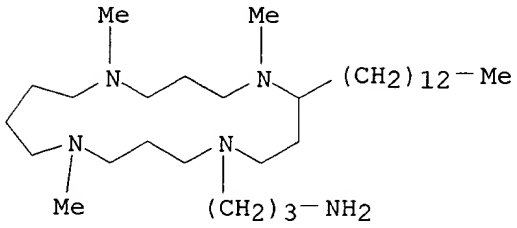
=> d l8 1 all

L8 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2003 ACS
RN 396117-44-5 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecane-5-propanamine, 1,9,13-trimethyl-8-tridecyl-, pentahydrochloride (9CI) (CA INDEX NAME)
OTHER NAMES:
CN SL 11239
MF C32 H69 N5 . 5 Cl H
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

CRN (395649-55-5)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C13N4	NC3NC3NC3NC4	17	C13N4	4584.21.1	1



●5 HCl

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1

AN 136:167548 CA
TI Synthesis of cyclic polyamine analogs for cancer therapy
IN Frydman, Benjamin; Hesse, Manfred; Guggisberg, Armin; Popaj, Kasmin; Drandarov, Konstantin; Basu, Hirak; Bhattacharya, Subhra; Wang, Yu
PA Slil Biomedical Corporation, USA
SO PCT Int. Appl., 105 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D257-02
ICS C07D255-02; A61K031-395; A61P035-00
CC 31-6 (Alkaloids)
Section cross-reference(s): 1
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002010142	A1	20020207	WO 2001-US24282	20010802

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2000-222522P 20000802
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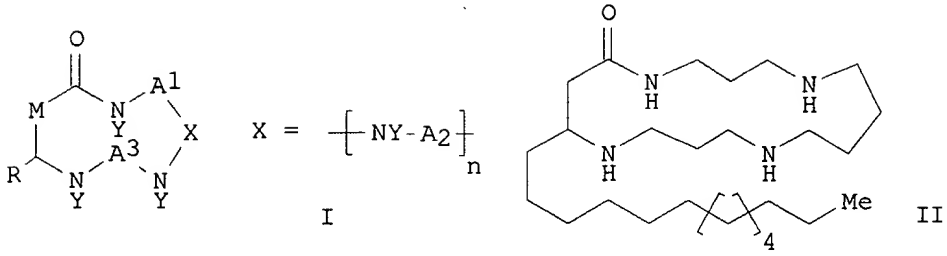


I II

AB Novel cyclic polyamine compds., such as I [A1, A2 = C1-C8 alkyl; Y = H, C1-C4 alkyl; M = C1-C4 alkyl; n = 0-3; R = C1-C32 alkyl], as well as all stereoisomers and salts thereof, were prepd. for treating diseases caused by uncontrolled proliferation of cells, such as cancer, esp. prostate cancer, and for inducing intracellular ATP hydrolysis for treatment of other disorders. Thus, cyclic polyamine II was prepd. via multistep synthetic sequence starting from triphenylphosphine, Et bromoacetate, myristylaldehyde and spermine. II.3HCl showed ID50 = 0.83.mu.M on prostate tumor cell growth.

ST polyamine cyclic prepn anticancer budmunchiamine

IT Polyamines
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(analog; prepn. of cyclic polyamine analogs for cancer therapy)

IT Cyclization
(lactamization, macrolactamization; in prepn. of cyclic polyamine analogs for cancer therapy)

IT Macrocyclization
(macrolactamization; in prepn. of cyclic polyamine analogs for cancer therapy)

IT Prostate gland
(neoplasm, inhibitors; prepn. of cyclic polyamine analogs for cancer therapy)

IT Cytotoxicity
(of cyclic polyamine analogs on survival of DuPro cells)

IT Alkylation
(of secondary amino groups in prepn. of cyclic polyamine analogs for cancer therapy)

IT Peptides, biological studies
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pentapeptides; prepn. of cyclic polyamine analogs for cancer therapy)

IT Antitumor agents
(prostate gland; prepn. of cyclic polyamine analogs for cancer therapy)

IT Peptides, biological studies
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(tetrapeptides; prepn. of cyclic polyamine analogs for cancer therapy)

IT 56-65-5, ATP, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(hydrolysis; in a cancerous cell via cyclic polyamine analogs)

IT 4375-83-1, Tris(dimethylamino)borane
RL: RGT (Reagent); RACT (Reactant or reagent)
(in prepn. of cyclic polyamine analogs for cancer therapy)

IT 139750-76-8P 139750-77-9P 396117-44-5P, SL 11239 396117-45-6P, SL 11238 396117-46-7P, SL 11174 396117-47-8P, SL 11197 396117-48-9P, SL 11199 396117-49-0P, SL 11200 396117-50-3P, SL 11208
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

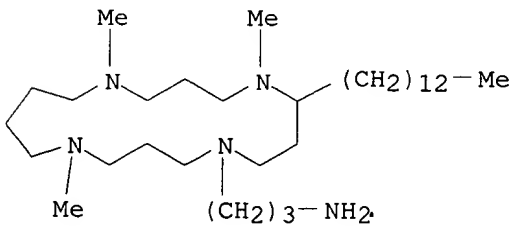
(prepn. of cyclic polyamine analogs for cancer therapy)
IT 395649-52-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of cyclic polyamine analogs for cancer therapy)
IT 110-60-1P, Putrescine 124-20-9P, Spermidine
RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of cyclic polyamine analogs for cancer therapy)
IT 50-00-0, Formalin, reactions 71-44-3, Spermine 105-36-2, Ethyl bromoacetate 107-13-1, Acrylonitrile, reactions 112-31-2, Caprinaldehyde 112-54-9, Laurinaldehyde 124-25-4, Myristinaldehyde 603-35-0, Triphenylphosphine, reactions 73453-98-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of cyclic polyamine analogs for cancer therapy)
IT 1530-45-6P 28290-90-6P 38112-60-6P 42778-95-0P 75814-58-3P 135251-95-5P 139750-78-0P, Budmunchiamine C 335153-35-0P 335153-39-4P 335153-41-8P 335153-43-0P 395649-49-7P 395649-50-0P 395649-51-1P 395649-53-3P 395649-54-4P 395649-55-5P 395649-56-6P 395649-57-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of cyclic polyamine analogs for cancer therapy)
IT 10433-06-4, Antimony(III)ethoxide 25895-60-7, Sodium cyanoborohydride
RL: RGT (Reagent); RACT (Reactant or reagent)
(prepn. of cyclic polyamine analogs for cancer therapy)
RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Squibb Bristol Myers Co; EP 0451547 A 1991 CAPLUS
(2) Univ Hawaii; EP 0792875 A 1997 CAPLUS

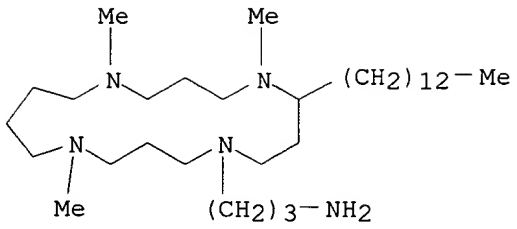
=> d l8 2 all

L8 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2003 ACS
RN 395649-55-5 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecane-5-propanamine, 1,9,13-trimethyl-8-tridecyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C32 H69 N5
CI COM
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C13N4	NC3NC3NC3NC4	17	C13N4	4584.21.1	1





Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1	pH 1	(1) ACD
Bioconc. Factor (BCF)	1	pH 4	(1) ACD
Bioconc. Factor (BCF)	1	pH 7	(1) ACD
Bioconc. Factor (BCF)	3.78	pH 8	(1) ACD
Bioconc. Factor (BCF)	419479	pH 10	(1) ACD
Boiling Point (BP)	595.8+/-50.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	88.78+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	308.7+/-44.8 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	16		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	2		(1) ACD
Koc (KOC)	1	pH 1	(1) ACD
Koc (KOC)	1	pH 4	(1) ACD
Koc (KOC)	1	pH 7	(1) ACD
Koc (KOC)	1.81	pH 8	(1) ACD
Koc (KOC)	200599	pH 10	(1) ACD
logD (LOGD)	0.92	pH 1	(1) ACD
logD (LOGD)	0.93	pH 4	(1) ACD
logD (LOGD)	1.86	pH 7	(1) ACD
logD (LOGD)	2.95	pH 8	(1) ACD
logD (LOGD)	7.99	pH 10	(1) ACD
logP (LOGP)	8.923+/-0.454		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	523.92		(1) ACD
pKa (PKA)	10.45+/-0.10	Most Basic	(1) ACD
Vapor Pressure (VP)	3.67E-14 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD)

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1

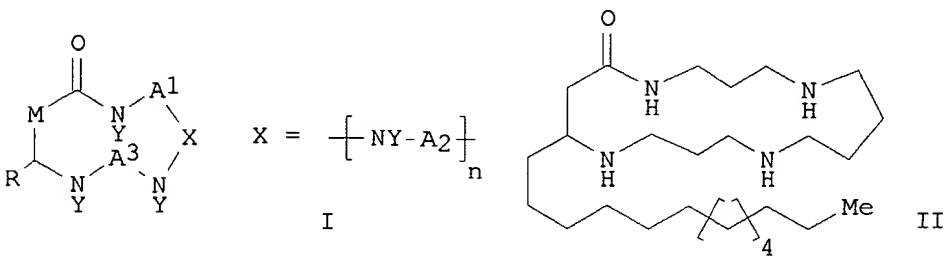
AN 136:167548 CA
TI Synthesis of cyclic polyamine analogs for cancer therapy
IN Frydman, Benjamin; Hesse, Manfred; Guggisberg, Armin; Popaj, Kasmin; Drandarov, Konstantin; Basu, Hirak; Bhattacharya, Subhra; Wang, Yu
PA Slil Biomedical Corporation, USA

SO PCT Int. Appl., 105 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D257-02
ICS C07D255-02; A61K031-395; A61P035-00
CC 31-6 (Alkaloids)
Section cross-reference(s): 1
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002010142	A1	20020207	WO 2001-US24282	20010802

PI W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2000-222522P 20000802
GI



AB Novel cyclic polyamine compds., such as I [A1, A2 = C1-C8 alkyl; Y = H, C1-C4 alkyl; M = C1-C4 alkyl; n = 0-3; R = C1-C32 alkyl], as well as all stereoisomers and salts thereof, were prepd. for treating diseases caused by uncontrolled proliferation of cells, such as cancer, esp. prostate cancer, and for inducing intracellular ATP hydrolysis for treatment of other disorders. Thus, cyclic polyamine II was prepd. via multistep synthetic sequence starting from triphenylphosphine, Et bromoacetate, myristylaldehyde and spermine. II.3HCl showed ID50 = 0.83.mu.M on prostate tumor cell growth.

ST polyamine cyclic prepn anticancer budmunchiamine
IT Polyamines
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(analog; prepn. of cyclic polyamine analogs for cancer therapy)
IT Cyclization
(lactamization, macrolactamization; in prepn. of cyclic polyamine analogs for cancer therapy)
IT Macrocyclization
(macrolactamization; in prepn. of cyclic polyamine analogs for cancer therapy)
IT Prostate gland
(neoplasm, inhibitors; prepn. of cyclic polyamine analogs for cancer therapy)
IT Cytotoxicity

(of cyclic polyamine analogs on survival of DuPro cells)
IT Alkylation
(of secondary amino groups in prepn. of cyclic polyamine analogs for cancer therapy)
IT Peptides, biological studies
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pentapeptides; prepn. of cyclic polyamine analogs for cancer therapy)
IT Antitumor agents
(prostate gland; prepn. of cyclic polyamine analogs for cancer therapy)
IT Peptides, biological studies
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(tetrapeptides; prepn. of cyclic polyamine analogs for cancer therapy)
IT 56-65-5, ATP, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(hydrolysis; in a cancerous cell via cyclic polyamine analogs)
IT 4375-83-1, Tris(dimethylamino)borane
RL: RGT (Reagent); RACT (Reactant or reagent)
(in prepn. of cyclic polyamine analogs for cancer therapy)
IT 139750-76-8P 139750-77-9P 396117-44-5P, SL 11239 396117-45-6P, SL 11238 396117-46-7P, SL 11174 396117-47-8P, SL 11197 396117-48-9P, SL 11199 396117-49-0P, SL 11200 396117-50-3P, SL 11208
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of cyclic polyamine analogs for cancer therapy)
IT 395649-52-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of cyclic polyamine analogs for cancer therapy)
IT 110-60-1P, Putrescine 124-20-9P, Spermidine
RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of cyclic polyamine analogs for cancer therapy)
IT 50-00-0, Formalin, reactions 71-44-3, Spermine 105-36-2, Ethyl bromoacetate 107-13-1, Acrylonitrile, reactions 112-31-2, Caprinaldehyde 112-54-9, Laurinaldehyde 124-25-4, Myristinaldehyde 603-35-0, Triphenylphosphine, reactions 73453-98-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of cyclic polyamine analogs for cancer therapy)
IT 1530-45-6P 28290-90-6P 38112-60-6P 42778-95-0P 75814-58-3P 135251-95-5P 139750-78-0P, Budmunchiamine C 335153-35-0P 335153-39-4P 335153-41-8P 335153-43-0P 395649-49-7P 395649-50-0P 395649-51-1P 395649-53-3P 395649-54-4P 395649-55-5P 395649-56-6P 395649-57-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of cyclic polyamine analogs for cancer therapy)
IT 10433-06-4, Antimony(III)ethoxide 25895-60-7, Sodium cyanoborohydride
RL: RGT (Reagent); RACT (Reactant or reagent)
(prepn. of cyclic polyamine analogs for cancer therapy)
RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Squibb Bristol Myers Co; EP 0451547 A 1991 CAPLUS
(2) Univ Hawaii; EP 0792875 A 1997 CAPLUS

=> d his

(FILE 'HOME' ENTERED AT 12:58:18 ON 18 MAR 2003)

FILE 'REGISTRY' ENTERED AT 12:58:26 ON 18 MAR 2003
L1 STRUCTURE UPLOADED

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L2              QUE L1
L3            0 S L1 EXA SAM
L4            0 S L1 FAM SAM
L5            2 S L1 SSS SAM
L6              STRUCTURE UPLOADED
L7              QUE L6
L8            2 S L6 SSS FULL

=> e spermi
E1            8     SPERMATURIN/BI
E2            1     SPERMETHRIN/BI
E3            3 --> SPERMI/BI
E4           11     SPERMIA/BI
E5            9     SPERMIC/BI
E6            1     SPERMICI/BI
E7            1     SPERMICIDE/BI
E8            1     SPERMICIDI/BI
E9            1     SPERMICIDIN/BI
E10           2     SPERMID/BI
E11           1     SPERMIDI/BI
E12           1     SPERMIDIC/BI

=> e spermidine
E1            1     SPERMIDIC/BI
E2          506     SPERMIDIN/BI
E3         2411 --> SPERMIDINE/BI
E4            4     SPERMIDINE:PUTRESCINE/BI
E5           26     SPERMIDINIUM/BI
E6            1     SPERMIDINO/BI
E7            1     SPERMIDOSE/BI
E8            1     SPERMIF/BI
E9            1     SPERMIFOL/BI
E10           1     SPERMIFOLIUM/BI
E11          31     SPERMIN/BI
E12           1     SPERMINDI/BI

=> s e3
L9         2411 SPERMIDINE/BI

=> e spermine
E1            1     SPERMINDI/BI
E2            1     SPERMINDIOL/BI
E3          261 --> SPERMINE/BI
E4            1     SPERMINE:SPERMIDINE/BI
E5            1     SPERMINECARBOX/BI
E6            1     SPERMINECARBOXAMIDO/BI
E7            3     SPERMININ/BI
E8           11     SPERMININE/BI
E9            3     SPERMININIUM/BI
E10           6     SPERMINIUM/BI
E11           1     SPERMINOGEN/BI
E12           1     SPERMINON/BI

=> s e3-e4
            261 SPERMINE/BI
              1 "SPERMINE:SPERMIDINE"/BI
L10         262 (SPERMINE/BI OR "SPERMINE:SPERMIDINE"/BI)

=> e budmunchimine
E1           22     BUDMUNCHI/BI
E2           22     BUDMUNCHIAMINE/BI
E3            0 --> BUDMUNCHIMINE/BI
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E4            1     BUDO/BI
E5            2     BUDOFFICIDE/BI
E6            1     BUDOFORM/BI
E7           12     BUDORCAS/BI
E8            1     BUDORM/BI
E9            1     BUDOTITANE/BI
E10          11     BUDR/BI
E11           2     BUDRAL/BI
E12           2     BUDRALAZIN/BI

=> s e1-e2
            22 BUDMUNCHI/BI
            22 BUDMUNCHIAMINE/BI
L11         22 (BUDMUNCHI/BI OR BUDMUNCHIAMINE/BI)

=> d l9 2411 all

L9   ANSWER 2411 OF 2411  REGISTRY  COPYRIGHT 2003 ACS
RN   56-18-8  REGISTRY
CN   1,3-Propanediamine, N-(3-aminopropyl)- (9CI)  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN   Dipropylamine, 3,3'-diamino- (6CI, 8CI)
OTHER NAMES:
CN   1,5,9-Triazanonane
CN   1,7-Diamino-4-azaheptane
CN   1-Propanamine, 3,3'-iminobis-
CN   3,3'-Diaminodipropylamine
CN   3,3'-Iminobis(propylamine)
CN   3,3'-Iminodi(propylamine)
CN   4-Aza-1,7-diaminoheptane
CN   4-Azaheptamethylenediamine
CN   4-Azaheptane-1,7-diamine
CN   Bis(3-aminopropyl)amine
CN   Caldine
CN   Di(3-aminopropyl)amine
CN   Dipropylenetriamine
CN   N-(3-Aminopropyl)-1,3-propanediamine
CN   N-3-Aminopropyl-1,3-diaminopropane
CN   Norspermidine
CN   P 2 (hardener)
CN   sym-Norspermidine
FS   3D CONCORD
MF   C6 H17 N3
CI   COM
LC   STN Files:   AGRICOLA, ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS,
       BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CHEMCATS,
       CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, DDFU, DETHERM*, DRUGU, EMBASE,
       GMELIN*, HODOC*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MSDS-OHS, NAPRALERT,
       NIOSHTIC, PHAR, PROMT, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, TULSA,
       USPAT2, USPATFULL
         (*File contains numerically searchable property data)
     Other Sources:   DSL**, EINECS**, TSCA**
         (**Enter CHEMLIST File for up-to-date regulatory information)
```

$H_2N-(CH_2)_3-NH-(CH_2)_3-NH_2$

Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1	pH 1	(1) ACD
Bioconc. Factor (BCF)	1	pH 4	(1) ACD
Bioconc. Factor (BCF)	1	pH 7	(1) ACD
Bioconc. Factor (BCF)	1	pH 8	(1) ACD
Bioconc. Factor (BCF)	1	pH 10	(1) ACD
Boiling Point (BP)	242.1+/-0.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	47.91+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	118.3+/-0.0 deg C		(1) ACD
H acceptors (HAC)	3		(1) ACD
H donors (HD)	5		(1) ACD
Koc (KOC)	1	pH 1	(1) ACD
Koc (KOC)	1	pH 4	(1) ACD
Koc (KOC)	1	pH 7	(1) ACD
Koc (KOC)	1	pH 8	(1) ACD
Koc (KOC)	1	pH 10	(1) ACD
logD (LOGD)	-7.14	pH 1	(1) ACD
logD (LOGD)	-7.14	pH 4	(1) ACD
logD (LOGD)	-6.56	pH 7	(1) ACD
logD (LOGD)	-5.41	pH 8	(1) ACD
logD (LOGD)	-2.07	pH 10	(1) ACD
logP (LOGP)	-1.143+/-0.245		(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	131.22		(1) ACD
pKa (PKA)	10.71+/-0.20	Most Basic	(1) ACD
Vapor Pressure (VP)	0.0346223 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

1289 REFERENCES IN FILE CA (1962 TO DATE)
277 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1294 REFERENCES IN FILE CAPLUS (1962 TO DATE)
48 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1

AN 138:175938 CA
TI One-part self-priming dental adhesive containing polymerizable (meth)acrylamide
IN Klee, Joachim E.; Walz, Uwe
PA Dentsply International Inc., USA
SO PCT Int. Appl., 17 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K006-00
ICS A61K006-083
CC 63-7 (Pharmaceuticals)
Section cross-reference(s): 37
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003013444	A1	20030220	WO 2002-US25005	20020806
	W: CA, JP, SE				

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR

PRAI US 2001-311433P 20010810
US 2002-213303 20020806

AB A dental adhesive compn. for bonding dental restoratives to dentin and enamel provides a 1-part self-etching, self-priming dental adhesive compn. having hydrolysis stable polymerizable acidic adhesive monomers. Thus, bis(3-methacryloylamidopropyl)diethylphosphonic acid was prepd. by the reaction of bis(3-aminopropyl)amine with methacrylic acid in the presence of dimethylaminopyridine, and DCC in CH2Cl2 and acetone, followed by the addn. of diethylphosphonic acid Et ester and hydrolysis.

ST selfpriming dental dental adhesive polymerizable methacrylamide prepn

IT Dental materials and appliances
(adhesives; one-part self-priming dental adhesive contg. polymerizable (meth)acrylamide)

IT Pigments, nonbiological
Polymerization catalysts
Polymerization inhibitors
Stabilizing agents
(one-part self-priming dental adhesive contg. polymerizable (meth)acrylamide)

IT Polymerization catalysts
(photopolymn.; one-part self-priming dental adhesive contg. polymerizable (meth)acrylamide)

IT Polymerization catalysts
(redox; one-part self-priming dental adhesive contg. polymerizable (meth)acrylamide)

IT Polymerization catalysts
(thermal; one-part self-priming dental adhesive contg. polymerizable (meth)acrylamide)

IT 56-18-8, Bis(3-aminopropyl)amine 78-40-0 79-41-4, Methacrylic acid, reactions 682-30-4, Diethyl vinylphosphonate 920-46-7, Methacryloyl chloride 929-59-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(in polymerizable (meth)acrylamide prepn.; one-part self-priming dental adhesive contg. polymerizable (meth)acrylamide)

IT 497222-54-5P 497222-55-6P 497222-57-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(in polymerizable (meth)acrylamide prepn.; one-part self-priming dental adhesive contg. polymerizable (meth)acrylamide)

IT 64-17-5, Ethanol, uses 67-64-1, Acetone, uses 75-65-0, uses
RL: NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); PYP (Physical process); PROC (Process); USES (Uses)
(one-part self-priming dental adhesive contg. polymerizable (meth)acrylamide)

IT 497222-56-7P 497222-58-9P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(one-part self-priming dental adhesive contg. polymerizable (meth)acrylamide)

IT 128-37-0, 2,6-Di-tert-butyl-p-cresol, biological studies 150-76-5, Hydroquinone monomethyl ether 5117-13-5 5441-99-6 7283-61-6 13886-05-0 497222-59-0 497222-60-3 497222-61-4 497222-62-5 497222-63-6 497222-64-7 497222-65-8 497222-66-9 497222-67-0 497222-68-1 497222-69-2 497222-70-5 497222-71-6 497222-72-7 497222-73-8 497222-74-9 497222-75-0
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(one-part self-priming dental adhesive contg. polymerizable (meth)acrylamide)

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD

(1) Akahane, S; US 6174935 B1 2001 CAPLUS

(2) Erdmann, C; WO 0202057 A 2002
(3) Kuraray Co; EP 1057468 A 2000 CAPLUS
(4) Moszner, N; US 2002016384 A1 2002 CAPLUS
(5) Ohno, H; US 5925690 A 1999 CAPLUS
(6) Tokuyama Corp; EP 0811368 A 1997 CAPLUS

REFERENCE 2

AN 138:161371 CA
TI Lightweight and small-sized plasma trap made of porous ceramics for plasma treatment apparatus
IN Suzuki, Kenji; Uemoto, Hideo; Shimai, Shunzo; Matsuyama, Kazushi; Ichijima, Masahiko
PA Toshiba Ceramics Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
IC ICM C23C016-50
ICS B01J019-08; C04B038-00; H01L021-205
CC 75-1 (Crystallography and Liquid Crystals)
Section cross-reference(s): 57, 76
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 2003041368	A2	20030213	JP 2001-230942	20010731
PRAI JP 2001-230942		20010731		

AB The plasma trap, for inactivating plasma leaked from a plasma reaction chamber, is disposed at an inlet and/or an outlet of feeding gases, and is made of porous ceramics with porosity 40-90% contg. three-dimensional continuous open pores. The plasma trap has low pressure loss and high thermal shock resistance and can flow a large amt. of gases.
ST plasma trap porous ceramic; CVD plasma trap porous ceramic
IT Epoxy resins, uses
RL: TEM (Technical or engineered material use); USES (Uses)
(gelating agent; in prepn. of porous ceramics having continuous open pores for plasma traps for plasma treatment app.)
IT Vapor deposition apparatus
(plasma; plasma trap made of porous ceramics having continuous open pores for plasma treatment app.)
IT Ceramics
(porous; plasma trap made of porous ceramics having continuous open pores for plasma treatment app.)
IT Plasma
(traps for; plasma trap made of porous ceramics having continuous open pores for plasma treatment app.)
IT 1344-28-1, Alumina, uses
RL: TEM (Technical or engineered material use); USES (Uses)
(ceramics; plasma trap made of porous ceramics having continuous open pores for plasma treatment app.)
IT 56-18-8
RL: RCT (Reactant); TEM (Technical or engineered material use); RACT (Reactant or reagent); USES (Uses)
(crosslinking agent for epoxy resin; in prepn. of porous ceramics having continuous open pores for plasma traps for plasma treatment app.)
IT 9003-03-6, Ammonium polyacrylate
RL: TEM (Technical or engineered material use); USES (Uses)
(dispersing agent; in prepn. of porous ceramics having continuous open pores for plasma traps for plasma treatment app.)
IT 139-96-8, Triethanolamine laurylsulfate
RL: TEM (Technical or engineered material use); USES (Uses)

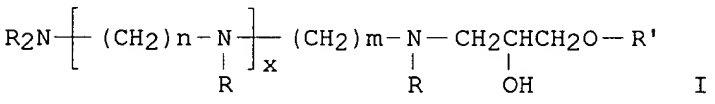
(foaming agent; in prepn. of porous ceramics having continuous open pores for plasma traps for plasma treatment app.)

REFERENCE 3

AN 138:124243 CA
TI Production of alkyl glycidyl ether-capped polyamine antifoaming agents
IN Sassano, Slone Caroline; Lassila, Kevin Rodney
PA Air Products and Chemicals, Inc., USA
SO Eur. Pat. Appl., 13 pp.
CODEN: EPXXDW
DT Patent
LA English
IC ICM C11D003-00
ICS C11D003-37
CC 46-4 (Surface Active Agents and Detergents)
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI EP 1277829	A2	20030122	EP 2002-15652	20020716
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
PRAI US 2001-909555	20010720			

GI



I

AB The foaming of an aq. compn. or an industrial process is controlled by the incorporation of a foam controlling agent having the general formula (I), where n and m are 2 or 3, x is 1-6, R is hydrogen or -CH2-CH(OH)-CH2-O-R', and R' is a C4-C22-alkyl group, the compd. I being capable of generating an initial foam height at least 30% less than a 0.1% aq. soln. of dioctyl sodium sulfosuccinate (DOSS) when added at 0.1% to the DOSS soln. The alkyl glycidyl ether-capped polyamine antifoaming agents can be used in water-thinned coating compns., inks, agricultural or adhesive compns., or in pulp and paper processing, wastewater treatment, textile dyeing and petroleum gas scrubbing. Thus, 1:1 adduct of diethylenetriamine and Bu glycidyl ether (BGE) was produced by adding one equiv. of BGE to diethylenetriamine at a rate allowing to keep the reaction mixt. temp. between 90 and 120.degree., followed by heating the mixt. at 100.degree. for 40 min.
ST nonpolymeric polyamine alkyl glycidyl ether deriv antifoaming agent prodn
IT Ethers, uses
RL: IMF (Industrial manufacture); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(glycidyl, C12-C16-alkyl, reaction products with nonpolymeric polyamines; prodn. of alkyl glycidyl ether-capped polyamine antifoaming agents)
IT Wetting agents
(nonionic; prodn. of alkyl glycidyl ether-capped polyamines suitable for use as)
IT Amines, uses
RL: IMF (Industrial manufacture); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(polyamines, nonpolymeric, reaction products with alkyl glycidyl

ethers; prodn. of alkyl glycidyl ether-capped polyamine antifoaming agents)

IT Antifoaming agents
Surfactants
(prodn. of alkyl glycidyl ether-capped polyamine antifoaming agents)

IT 56-18-8DP, reaction products with alkyl glycidyl ethers 112-24-3DP, reaction products with alkyl glycidyl ethers 63888-68-6P 488783-16-0P 488783-17-1P 488783-18-2P 488783-19-3P 488783-20-6P 488783-21-7P 488803-37-8P 490035-26-2P 490035-27-3P 490035-28-4P 490035-29-5P 490035-30-8P 491577-26-5P 491577-27-6P 491577-28-7P 491577-29-8P 491577-30-1P 491577-31-2P 491577-32-3P 491577-33-4P
RL: IMF (Industrial manufacture); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(prodn. of alkyl glycidyl ether-capped polyamine antifoaming agents)

IT 56-18-8, Di(3-aminopropyl)amine 111-40-0, Diethylenetriamine 112-24-3, Ancamine TETA 2426-08-6, Epodil 741 2461-15-6, Epodil 746 160338-56-7, Epodil 748
RL: RCT (Reactant); RACT (Reactant or reagent)
(prodn. of alkyl glycidyl ether-capped polyamine antifoaming agents)

IT 577-11-7, Dioctyl sodium sulfosuccinate
RL: TEM (Technical or engineered material use); USES (Uses)
(suppression of foam of; prodn. of alkyl glycidyl ether-capped polyamine antifoaming agents)

REFERENCE 4

AN 138:99890 CA

TI New 3-D bimetallic magnetic compounds, [Ni(dipn)]3[M(CN)6]2.7H2O (MIII = Fe, Co; dipn = N,N-di(3-aminopropyl)amine)

AU Ohba, Masaaki; Yamada, Mitsuteru; Usuki, Naoki; Okawa, Hisashi

CS Department of Chemistry, Faculty of Science, Kyushu University, Fukuoka, 812-8581, Japan

SO Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals (2002), 379, 241-246
CODEN: MCLCE9; ISSN: 1058-725X

PB Taylor & Francis Ltd.

DT Journal

LA English

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 75, 77

AB New cyanide-bridged bimetallic compds., [Ni(dipn)]3[M(CN)6]2.7H2O (M = Fe (I), Co (II); dipn = N,N-di(3-aminopropyl)amine) were prepd. and their crystal structures and magnetic properties were investigated. They are isostructural. Crystal data of I: monoclinic, C2/c, a = 24.097(4), b = 14.344(3), c = 16.681(2) .ANG., .beta. = 100.57(1).degree., V = 5667(1) .ANG.3, Z = 4, .rho.c = 1.312 g/cm3, 4480 obsd. reflections with I > 3.sigma.(I), R = 0.059, Rw = 0.097; II: monoclinic, C2/c, a = 24.466(4), b = 14.534(3), c = 16.475(3) .ANG., .beta. = 100.04(1).degree., V = 5768(1) .ANG.3, Z = 4, .rho.c = 1.296 g/cm3, 2875 obsd. reflections with I > 3.sigma.(I), R = 0.057, Rw = 0.081. In the crystal of I each [Fe(CN)6]3- makes bond to 3 [Ni(dipn)]2- cations to form a 2D sheet and the 2D sheets are connected by [Ni(dipn)(H2O)]2+ cations providing a 3D network structure. Compd. I shows a ferromagnetic ordering in the bulk with TC = 7.8 K.

ST nickel aminopropylamine cyanoferrate cyanocobaltate prepn structure; crystal structure nickel aminopropylamine complex cyanoferrate cyanocobaltate; ferromagnetic ordering nickel aminopropylamine cyanoferrate

IT Ferromagnetic ordering
Magnetic susceptibility
Magnetization
(of nickel [bis(aminopropyl)amine]nickel 3-dimensional complex with

ferricyanide)
IT Crystal structure
Molecular structure
(of nickel [bis(aminopropyl)amine]nickel 3-dimensional complexes with ferricyanide/cobalticyanide)
IT 484008-56-2P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn., crystal and mol. structure of polymeric)
IT 484008-54-0P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(prepn., crystal and mol. structure, and ferromagnetic ordering in polymeric)
IT 56-18-8, Bis(3-aminopropyl)amine 13746-66-2, Tripotassium hexacyanoferrate(3-) 13963-58-1, Tripotassium hexacyanocobaltate(3-)
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for prepn. of nickel [bis(aminopropyl)amine]nickel complexes with ferricyanide/cobalticyanide)
RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
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(2) Ohba, M; Inorg Chem 1998, V37, P3349 CAPLUS
(3) Ohba, M; J Am Chem Soc 1994, V116, P11566 CAPLUS
(4) Ohba, M; J Am Chem Soc 1997, V119, P1011 CAPLUS
(5) Ohba, M; J Chem Soc, Dalton Trans 1997, P1733 CAPLUS

REFERENCE 5

AN 138:49001 CA
TI Nickel(II) and palladium(II) complexes with singly condensed diprimary triamines and 2-aminobenzaldehyde
AU Kwiatkowski, Edmund; Romanowski, Grzegorz; Suwinska, Kinga
CS Department of Chemistry, University of Gdansk, Gdansk, PL-80952, Pol.
SO Polyhedron (2002), 21(20), 2071-2079
CODEN: PLYHDE; ISSN: 0277-5387
PB Elsevier Science Ltd.
DT Journal
LA English
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 69, 73, 75
AB Six new nickel(II) and one palladium(II) complexes were obtained by complexation of unsym. Schiff bases HA, HD and HB resulting from 1:1 condensation of 2-aminobenzaldehyde with 1,5-diamino-3-azapentane, 1,7-diamino-4-azaheptane and 1,7-diamino-4-methyl-4-azaheptane, resp. NiAX (X = Cl, NO3, ClO4), NiBI, and Ni(HD)X2 (X = Cl, NO3) display an alternation of configuration at the metal center from planar through tetrahedrally-distorted planar to octahedral when going from A, through B, to D contg. complexes, as indicated by the variation in their spectroscopic and magnetic properties. NiAX complexes retain their planar structure in soln., whereas NiBI solns. show a weak paramagnetism in consequence of a rapid (on the NMR time-scale) equil. between low spin (S = 0) planar and high spin (S = 1) close to tetrahedral forms. Crystal structures of NiAClO4 and NiBI obtained by x-ray diffraction studies revealed a planar coordination in the former and a planar-to-tetrahedral distorted metal configuration with an angle between N1, Ni, N2 and N3, Ni, N4 planes of 41.degree. in the latter compd. An intermol. charge transfer transition accounting for an absorption of solid NiAClO4 in the 600-800 nm region, which is unusual for planar nickel(II) complexes, was postulated.
ST aminobenzaldehyde triamine Schiff nickel palladium complex prepn structure; crystal structure nickel aminobenzaldehyde triamine Schiff complex; thermodn isomerization nickel aminobenzaldehyde triamine Schiff complex; hydrogen bond nickel aminobenzaldehyde triamine Schiff complex

IT Transition metal complexes
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(Schiff base; prepn., crystal and mol. structure and photoacoustic spectra of nickel(II) and palladium(II) complexes of aminobenzaldehyde 1:1 Schiff bases with diaminoazapentane and diaminoazaheptanes)
IT Entropy
Free energy
Thermodynamics
(isomerization; of nickel(II) complex of aminobenzaldehyde 1:1 Schiff base with diaminoazaheptane)
IT Isomerization enthalpy
(of nickel(II) complex of aminobenzaldehyde 1:1 Schiff base with diaminoazaheptane)
IT Crystal structure
Hydrogen bond
Molecular structure
(of nickel(II) complexes of aminobenzaldehyde 1:1 Schiff bases with diaminoazapentane and diaminoazaheptane)
IT Charge transfer transition
Coordination sphere
Photoacoustic spectra
(of nickel(II) complexes of aminobenzaldehyde 1:1 Schiff bases with diaminoazapentane and diaminoazaheptanes)
IT Ligand field theory
(parameters; of nickel(II) complexes of aminobenzaldehyde 1:1 Schiff base with diaminoazaheptane)
IT Schiff bases
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(transition metal complexes; prepn., crystal and mol. structure and photoacoustic spectra of nickel(II) and palladium(II) complexes of aminobenzaldehyde 1:1 Schiff bases with diaminoazapentane and diaminoazaheptanes)
IT 478807-37-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and crystal and mol. structure and photoacoustic spectrum)
IT 478807-38-4P 478807-39-5P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and photoacoustic spectrum)
IT 478807-42-0P 478807-43-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and photoacoustic spectrum and ligand field parameters)
IT 478807-40-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 56-18-8, 1,7-Diamino-4-azaheptane 105-83-9,
1,7-Diamino-4-methyl-4-azaheptane 111-40-0, 1,5-Diamino-3-azapentane
529-23-7, 2-Aminobenzaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of nickel(II) and palladium(II) complexes of aminobenzaldehyde 1:1 Schiff bases with diaminoazapentane and diaminoazaheptanes)
IT 132953-33-4P 478807-45-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of nickel(II) and palladium(II) complexes of aminobenzaldehyde 1:1 Schiff bases with diaminoazapentane and diaminoazaheptanes)
IT 478807-44-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of nickel(II) and palladium(II) complexes of aminobenzaldehyde 1:1 Schiff bases with diaminoazapentane, diaminoazaheptane and diamino(methyl)azaheptane)
IT 478807-41-9P

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(prepn., crystal and mol. structure, photoacoustic spectrum and thermodn. of planar-tetrahedral equil.)

RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD
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REFERENCE 6

AN 138:40781 CA
TI Triphenyl boron addition product and its use as antifouling agent in coatings

IN Yoshimaru, Masaaki; Kohara, Masanori; Koga, Yuji
PA Yoshitomi Fine Chemicals Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
IC ICM C07F005-02
ICS A01K063-00; A01K075-00; A01K075-04; A01N037-32; A01N043-36; A01N047-14; A01N055-08; C09D005-16; C09D007-12; C09D183-04
CC 42-10 (Coatings, Inks, and Related Products)
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

PI JP 2002363187 A2 20021218 JP 2001-211385 20010607
PRAI JP 2001-211385 20010607
AB The patent relates to antifouling agent useful for fish nets, boat hulls, etc. wherein the antifouling agent is represented by (ph3B)-NH2R1-NH-R2-NH2-(Bph3) and its salts where R1 and R2 are the same or different C1-18 alkyl which may contain oxygen atom. Thus, di(triphenylboran)-3,3'-iminobis(propylamine) adduct prepd. by reacting triphenylboron sodium hydroxide salt soln. and 3,3'-iminobis(propylamine) was used as antifouling agent for fish nets and showed no bio-organism attachment after 6 mo.
ST antifouling agent triphenylboron iminobispropylamine addn product salt
IT Coating materials
(antifouling; prepn. of tri-Ph boron addn. product for antifouling coatings)
IT Antifouling agents
(prepn. of tri-Ph boron addn. product for antifouling coatings)
IT 478798-43-5P 478957-92-5P 478957-93-6P
RL: IMF (Industrial manufacture); RCT (Reactant); TEM (Technical or engineered material use); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(antifouling agent; prepn. of tri-Ph boron addn. product for antifouling coatings)
IT 56-18-8, 3,3'-Iminobis(propylamine) 79-10-7, Acrylic acid, reactions 1121-31-9, 2-Mercaptopyridine-N-oxide 12113-07-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(in prepn. of tri-Ph boron addn. product for antifouling coatings)

REFERENCE 7

AN 138:14687 CA
TI Strong monoarylide azo pigment/hydrocarbyl polypropylenepolyamine compositions, their production and their use
IN Hays, Byron G.
PA Engelhard Corporation, USA
SO U.S., 9 pp.
CODEN: USXXAM
DT Patent
LA English
IC ICM C09B029-01
ICS C09B029-00; C09B039-00
NCL 106496000
CC 41-3 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic Sensitizers)
Section cross-reference(s): 42
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6488759	B1	20021203	US 2001-940387	20010827

PRAI US 2001-940387 20010827
AB One aspect of the invention relates to tinctorially strong pigment compns. contg. a monoarylide pigment and a hydrocarbyl polypropylenepolyamine compd. [R(CH2CH2CH2NH)xH; R = C10-22-hydrocarbyl; x = 1-5]. Another aspect of the invention relates to making an azo pigment involving coupling a substituted or unsubstituted acetoacetanilide with at least one diazotized arom. amine in a soln. contg. a hydrocarbyl polypropyleneamine. The pigments may be used in paint, ink, electrostatic toner, powder coating, and paper compns. In an example, C.I. Pigment Yellow 65 with improved tinctorial strength was prepd. in the presence of tallow-alkyl tripropylenetetramine.
ST azo pigment prodn polypropylenepolyamine tinctorial effect improver
IT Pigments, nonbiological
(azo; prodn. of azo pigments in presence of polypropyleneamines for

improved tinctorial strength)

IT Alkyd resins
RL: TEM (Technical or engineered material use); USES (Uses)
(coatings; prodn. of azo pigments in presence of polypropyleneamines for improved tinctorial strength in)

IT Polyamines
RL: MOA (Modifier or additive use); USES (Uses)
(polyalkylene-; prodn. of azo pigments in presence of polypropyleneamines for improved tinctorial strength)

IT Coating materials
(prodn. of azo pigments in presence of polypropyleneamines for improved tinctorial strength in)

IT 92-15-9, Acetoacet-o-anisidide 93-68-5 93-70-9, Acetoacet-o-chloroanilide
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling component; prodn. of azo pigments in presence of polypropyleneamines for improved tinctorial strength)

IT 89-63-4, 4-Chloro-2-nitroaniline 96-96-8, 4-Methoxy-2-nitroaniline
RL: RCT (Reactant); RACT (Reactant or reagent)
(diazo component; prodn. of azo pigments in presence of polypropyleneamines for improved tinctorial strength)

IT 6371-96-6P, C.I. Pigment Orange 1
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(orange pigment; prodn. of azo pigments in presence of polypropyleneamines for improved tinctorial strength)

IT 56-18-8D, Dipropylenetriamine, N-tallow alkyl derivs. 109-76-2D, 1,3-Propylenediamine, N-tallow alkyl derivs. 4605-14-5D, Tripropylenetetramine, N-tallow alkyl derivs. 28872-01-7, N-Oleyldipropylenetriamine 32536-50-8, Stearyl tripropylenetetramine 45296-40-0, N-Stearyldipropylenetriamine 53731-85-4, N-Decyltripropylenetetramine 53853-64-8, N-Myristyltetrapropylenepentamine 67022-37-1, N-Lauryldipropylenetriamine 67228-82-4, N-Lauryltripropylenetetramine 67228-83-5 76287-08-6 86247-58-7, N-Myristyldipropylenetriamine 103956-02-1, Stearyl tetrapropylenepentamine 141097-26-9, N-Decyldipropylenetriamine 186038-73-3, N-Hexadecyltripropylenetetramine 209917-22-6, N-Hexadecyldipropylenetriamine 477284-51-8, N-Lauryltetrapropylenepentamine 477284-52-9, N-Decyltetrapropylenepentamine 477284-53-0, N-Myristyltripropylenetetramine 477284-54-1, N-Hexadecyltetrapropylenepentamine 477558-73-9, N-Isodecyltetrapropylenepentamine 477558-74-0, N-Isodecyltripropylenetetramine 477558-75-1, N-Isodecyldipropylenetriamine
RL: MOA (Modifier or additive use); USES (Uses)
(prodn. of azo pigments in presence of polypropyleneamines for improved tinctorial strength)

IT 6486-23-3P, C.I. Pigment Yellow 3 6528-34-3P, C.I. Pigment Yellow 65
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(yellow pigment; prodn. of azo pigments in presence of polypropyleneamines for improved tinctorial strength)

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD

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(2) Anon; EP 137630 1983 CAPLUS
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(12) Schwartz; US 5145997 A 1992 CAPLUS
(13) Stirling; US 5672202 A 1997 CAPLUS

REFERENCE 8

AN 138:10813 CA
TI Hydrothermal Synthesis and Structures of Three-Dimensional Zinc Phosphates Built-Up from Two-Dimensional Layers and One-Dimensional Chains and Ladders
AU Mandal, Sukhendu; Natarajan, Srinivasan
CS Framework Solids Laboratory, Chemistry and Physics of Materials Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, 560 064, India
SO Crystal Growth & Design (2002), 2(6), 665-673
CODEN: CGDEFU; ISSN: 1528-7483
PB American Chemical Society
DT Journal
LA English
CC 78-5 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 75
AB Three new Zn phosphates [(NH4)(CH3CH2CH2NH3)][Zn3(HPO4)(PO4)2] (I), [NH3(CH2)3NH(CH2)3NH3][Zn3(H2PO4)(HPO4)2(PO4)].cntdot.H2O (II), and [NH3(CH2)3NH2(CH2)3NH3][Zn3(HPO4)3(PO4)] (III), were synthesized in the presence of 1,3,5-triethylhexahydrotriazine (TEHT) and dipropylenetriamine (DPTA). Their structures were detd. by single-crystal x-ray diffraction. The structures consist of vertex-linking ZnO4 and PO4 tetrahedral units forming channels bound by 8-, 10-, and 16-T atoms (T = Zn, P). While the structures of I and II are built up from two-dimensional layers cross-linked by 1-dimensional ladders or chains, that of III is built up by crosslinking of ladders. The framework structure of II and III is built up from strictly alternating ZnO4 and PO4 units, and in I, infinite Zn-O-Zn chains are obsd., formed by two Zn atoms sharing two three-coordinated O atoms. The amine mol. in I, propylamine, was obtained by the decompn. of TEHT under hydrothermal conditions. The amine mols. in I-III occupy the channels. Crystal data: I, triclinic, space group = P(-1) (no. 2), M = 559.18, a 5.0986(6), b 10.4943(1), c 12.4457(1) .ANG., .alpha. 87.614(2), .beta. 87.258(1), .gamma. 89.994(2).degree., R1 = 0.0342, wR2 = 0.091 [1913 obsd. reflections with I > 2.sigma.(I)]; II, triclinic, space group = P(-1) (no. 2), M = 731.28, a 8.4821(7), b 9.1326(8), c 14.7961(1) .ANG., .alpha. 90.382(2), .beta. 100.123(2), .gamma. 107.04(1).degree., R1 = 0.0332, wR2 = 0.0747 [2954 obsd. reflections with I > 2.sigma.(I)] III, monoclinic, space group = Cc (no. 7), M = 713.26, a 15.1085(4), b 8.8403(4), c 17.2628(6) .ANG., .beta. 114.537(2).degree., R1 = 0.0315, wR2 = 0.0804 [2323 obsd. reflections with I > 2.sigma.(I)].
ST crystal structure zinc phosphate three dimensional; zinc phosphate three dimensional prepn structure
IT Crystal structure
Molecular structure
(of zinc phosphates with three dimensional structures)
IT 56-18-8, Dipropylenetriamine 7779-27-3
RL: NUU (Other use, unclassified); USES (Uses)
(for prepn. of three-dimensional zinc phosphates)
IT 7664-38-2, Phosphoric acid, reactions 14024-63-6, Bis(acetylacetonato)zinc
RL: RCT (Reactant); RACT (Reactant or reagent)
(for prepn. of three-dimensional zinc phosphates)
IT 476372-94-8P 476372-95-9P 476372-96-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(prepn. and crystal structure and thermal decompn. of three-dimensional zinc phosphates)

RE.CNT 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD
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REFERENCE 9

AN 137:389143 CA
TI Complexes for transferring therapeutic proteins and nucleic acids into an animal cell
IN Braun, Serge; Meyer, Olivier; Nazih, Abdesslame; Heissler, Denis
PA Transgene S.A., Fr.
SO PCT Int. Appl., 58 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07C271-20
ICS A61K048-00; C12N015-88
CC 63-6 (Pharmaceuticals)
Section cross-reference(s): 3, 23
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002092554	A1	20021121	WO 2002-EP5304	20020514

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI EP 2001-440134 20010515
US 2001-293188P 20010525

AB The present invention concerns new polar compds., complexes and compns. comprising them, wherein the compd. comprises: (i) a polar headgroup spacer, (ii) at least 1 hydrophobic moiety, and (iii) at least 1 hydrophilic polymer, and wherein the head-group spacer is coupled to the hydrophobic moiety and to the hydrophilic polymer. A lipid was prepd. by the reaction of PEG monomethyl ether with H2N(CH2)3N(BOC)(CH2)3N(BOC)(CH2)3N(BOC)(CH2)3NH2 followed by reaction with an aldehyde contg. oleoyl groups. A cationic lipid/DNA complex was obtained by the treatment of the above lipid with DNA.

ST therapeutic protein lipid animal cell; nucleic acid therapeutic lipid animal cell

IT Animal cell
Animal tissue culture
Drug delivery systems
Molecular weight distribution
Transformation, genetic
(complexes for transferring therapeutic proteins and nucleic acids into animal cell)

IT Nucleic acids
Proteins
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(complexes for transferring therapeutic proteins and nucleic acids into animal cell)

IT Lipids, biological studies
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(complexes, with DNA; complexes for transferring therapeutic proteins and nucleic acids into animal cell)

IT DNA

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(complexes, with lipids; complexes for transferring therapeutic proteins and nucleic acids into animal cell)

IT Polyoxyalkylenes, biological studies
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(derivs.; complexes for transferring therapeutic proteins and nucleic acids into animal cell)

IT 475976-05-7P, PcTG 238 475983-78-9P, PcTG 231
RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(complexes for transferring therapeutic proteins and nucleic acids into animal cell)

IT 608-66-2D, Dulcitol, derivs. 6917-36-8D, Pentitol, derivs. 7541-59-5D, Tetritol, derivs. 9003-39-8D, PVP, derivs. 9004-34-6D, Cellulose, derivs. 25322-68-3D, Polyethylene glycol, derivs. 37758-47-7D, Ganglioside GM1, derivs. 45007-61-2D, Hexitol, derivs. 158606-68-9D, Polyaspartamide, derivs.
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(complexes for transferring therapeutic proteins and nucleic acids into animal cell)

IT 56-18-8 107-13-1, 2-Propenenitrile, reactions 156-87-6, 1-Amino-3-propanol 598-21-0, Bromoacetyl bromide 9004-74-4, Polyethylene glycol monomethyl ether 24424-99-5, Di-tert-butyl dicarbonate 29655-46-7 61278-21-5 93790-78-4 475576-35-3 475576-36-4 475576-37-5 475576-38-6 475576-39-7 475576-40-0 475576-41-1 475576-42-2 475576-43-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(in prepn. of lipids contg. PEG; complexes for transferring therapeutic proteins and nucleic acids into animal cell)

IT 148983-25-9P 287973-38-0P 475576-28-4P 475576-29-5P 475576-30-8P 475576-31-9P 475576-32-0P 475576-33-1P 475576-34-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(in prepn. of lipids contg. PEG; complexes for transferring therapeutic proteins and nucleic acids into animal cell)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD

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(3) Valentis; WO 0040692 A 2000 CAPLUS

REFERENCE 10

AN 137:372547 CA
TI Anode catalyst containing metal complex for low-temperature fuel cell
IN Okada, Tatsuhiro; Suzuki, Yoshifumi; Hirose, Takashi; Ozawa, Takeo; Toda, Takako
PA Ministry of Economy, Trade and Industry; National Industrial Research Institute, Japan
SO Jpn. Kokai Tokkyo Koho, 12 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
IC ICM H01M004-90
ICS H01M004-92; H01M004-96; H01M008-10
CC 52-2 (Electrochemical, Radiational, and Thermal Energy Technology)
Section cross-reference(s): 67

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2002329500	A2	20021115	JP 2002-54597	20020228

PRAI JP 2001-58276 20010302

AB The title catalyst comprises a transition metal or its alloy and an org. metal complex having planar coordination structure. The catalyst is esp. suitable for polymer-electrolyte fuel cells and direct methanol fuel cells. Thus, a mixt. contg. [Pt(NH3)4]Cl2 and Co monoquinolyl phenylenediamine obtained by reacting 8-hydroxyquinoline, o-phenylenediamine, Na pyrosulfite, and Co acetate was heat treated with graphite particles to give an anode catalyst showing good MeOH oxidn. property and CO poisoning resistance.

ST anode catalyst transition metal complex planar coordination fuel cell

IT Catalysts
Fuel cell anodes
(anode catalyst contg. transition metal and metal complex having planar-coordination structure for low-temp. fuel cell)

IT Transition metals, uses
RL: CAT (Catalyst use); DEV (Device component use); USES (Uses)
(anode catalyst contg. transition metal and metal complex having planar-coordination structure for low-temp. fuel cell)

IT Fuel cells
(polymer electrolyte or direct methanol; anode catalyst contg. transition metal and metal complex having planar-coordination structure for low-temp. fuel cell)

IT 56-18-8D, N-(3-Aminopropyl)-1,3-propane diamine, complexes with cobalt 7440-48-4D, Cobalt, complexes with N-(3-Aminopropyl)-1,3-propanediamine 13933-32-9, Platinumtetraammine dichloride 14172-90-8 28903-71-1 53277-08-0
RL: CAT (Catalyst use); DEV (Device component use); USES (Uses)
(anode catalyst contg. transition metal and metal complex having planar-coordination structure for low-temp. fuel cell)

IT 7439-89-6DP, Iron, monoquinolylphenylenediamine complexes 7439-96-5DP, Manganese, monoquinolylphenylenediamine complexes 7440-02-0DP, Nickel, monoquinolylphenylenediamine complexes 7440-05-3DP, Palladium, monoquinolylphenylenediamine complexes 7440-48-4DP, Cobalt, monoquinolylphenylenediamine complexes 7440-50-8DP, Copper, monoquinolylphenylenediamine complexes 7440-62-2DP, Vanadium, monoquinolylphenylenediamine complexes
RL: CAT (Catalyst use); DEV (Device component use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(anode catalyst contg. transition metal and metal complex having planar-coordination structure for low-temp. fuel cell)

IT 7782-42-5, Graphite, uses
RL: CAT (Catalyst use); DEV (Device component use); USES (Uses)
(catalyst contg.; anode catalyst contg. transition metal and metal complex having planar-coordination structure for low-temp. fuel cell)

IT 7440-44-0, Glassy carbon, uses
RL: CAT (Catalyst use); DEV (Device component use); USES (Uses)
(glassy or activated, catalyst contg.; anode catalyst contg. transition metal and metal complex having planar-coordination structure for low-temp. fuel cell)

IT 95-54-5, o-Phenylenediamine, reactions 148-24-3, 8-Hydroxyquinoline, reactions 7681-57-4, Sodium pyrosulfite
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of; in prepn. of metal complex for fuel-cell anode catalyst)

=> d his

(FILE 'HOME' ENTERED AT 12:58:18 ON 18 MAR 2003)

FILE 'REGISTRY' ENTERED AT 12:58:26 ON 18 MAR 2003
L1 STRUCTURE UPLOADED
L2 QUE L1

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L3              0 S L1 EXA SAM
L4              0 S L1 FAM SAM
L5              2 S L1 SSS SAM
L6                STRUCTURE UPLOADED
L7                QUE L6
L8              2 S L6 SSS FULL
                  E SPERMI
                  E SPERMIDINE
L9           2411 S E3
                  E SPERMINE
L10           262 S E3-E4
                  E BUDMUNCHIMINE
L11            22 S E1-E2

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MISSING OPERATOR

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L11  ANSWER 1 OF 22  REGISTRY  COPYRIGHT 2003 ACS
RN   195734-30-6  REGISTRY
CN   1,5,9,13-Tetraazacycloheptadecan-6-one, 8-(11-pentadecenyl)-, (+)- (9CI)
     (CA INDEX NAME)
OTHER NAMES:
CN   (+)-Budmunchiamine L6
CN   Budmunchiamine L 6
FS   STEREOSEARCH
MF   C28 H56 N4 O
SR   CA
LC   STN Files:   CA, CAPLUS

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Currently available stereo shown.
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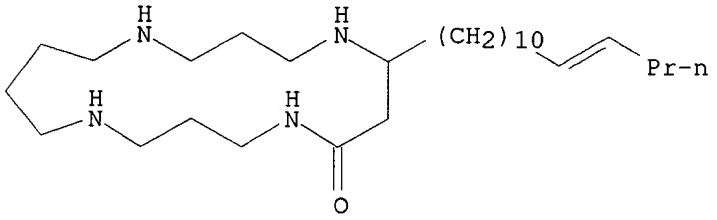


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              1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L11  ANSWER 2 OF 22  REGISTRY  COPYRIGHT 2003 ACS
RN   195734-29-3  REGISTRY
CN   1,5,9,13-Tetraazacycloheptadecan-6-one, 8-(13-heptadecenyl)-, (+)- (9CI)
     (CA INDEX NAME)
OTHER NAMES:
CN   (+)-Budmunchiamine L5
CN   Budmunchiamine L 5
FS   STEREOSEARCH
MF   C30 H60 N4 O
SR   CA
LC   STN Files:   BIOSIS, CA, CAPLUS
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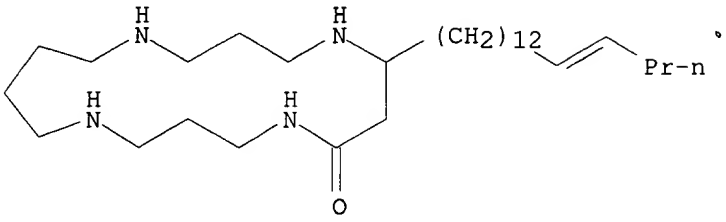
Rotation (+).
Double bond geometry unknown.
Currently available stereo shown.



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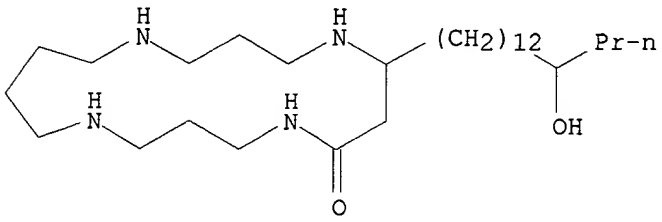
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L11 ANSWER 3 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 195734-28-2 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 8-(13-hydroxyhexadecyl)-, (+)-
(9CI) (CA INDEX NAME)
OTHER NAMES:
CN **(+)-Budmunchiamine L4**
CN **Budmunchiamine L 4**
FS STEREOSEARCH
MF C29 H60 N4 O2
SR CA
LC STN Files: BIOSIS, CA, CAPLUS

Rotation (+).
Currently available stereo shown.



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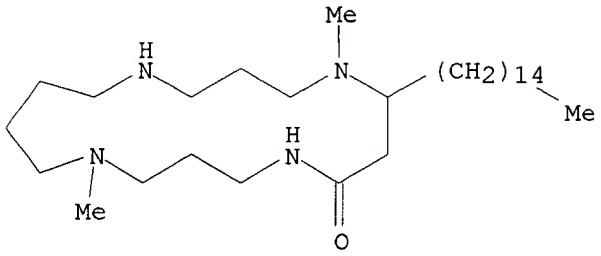
L11 ANSWER 4 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 180285-78-3 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 1,9-dimethyl-8-pentadecyl-, (-)-
(9CI) (CA INDEX NAME)
OTHER NAMES:
CN **9-Normethylbudmunchiamine K**
FS STEREOSEARCH
MF C30 H62 N4 O
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Rotation (-).
Currently available stereo shown.



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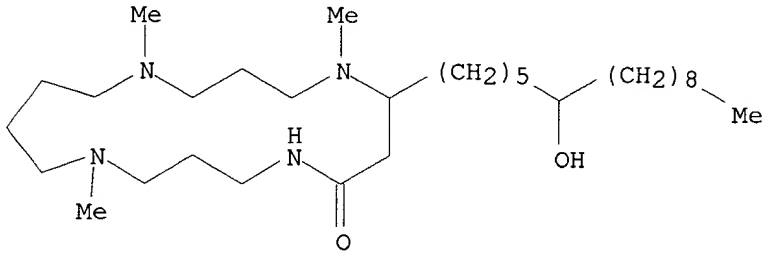
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L11 ANSWER 5 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 180285-72-7 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 8-(6-hydroxypentadecyl)-1,9,13-trimethyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **6'.xi.-Hydroxybudmunchiamine K**
FS STEREOSEARCH
MF C31 H64 N4 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Rotation (-).
Currently available stereo shown.



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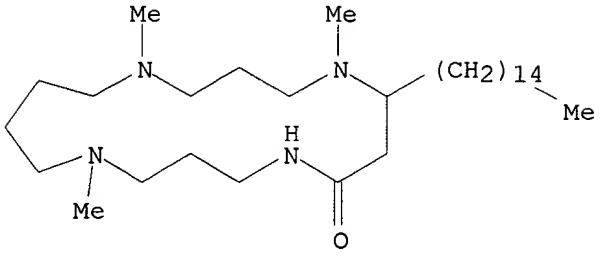
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L11 ANSWER 6 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 178494-87-6 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 1,9,13-trimethyl-8-pentadecyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine K**
MF C31 H64 N4 O
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Currently available stereo shown.



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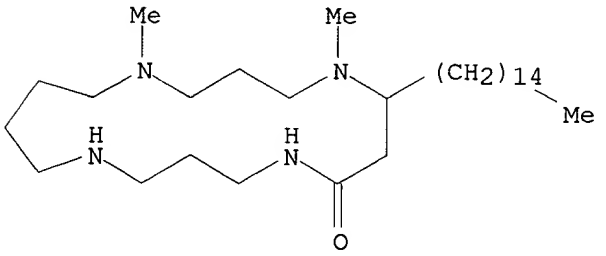
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L11 ANSWER 7 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 178494-86-5 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 9,13-dimethyl-8-pentadecyl-, (-)-
(9CI) (CA INDEX NAME)
OTHER NAMES:
CN **14-Normethylbudmunchiamine K**
FS STEREOSEARCH
MF C30 H62 N4 O
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Rotation (-).
Currently available stereo shown.



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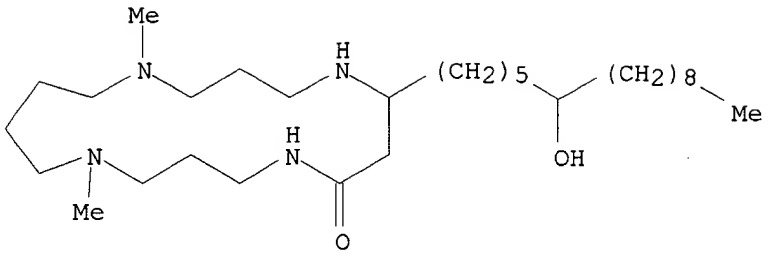
L11 ANSWER 8 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 178494-85-4 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 8-(6-hydroxypentadecyl)-1,13-
dimethyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **6'.xi.-Hydroxy-5-normethylbudmunchiamine K**
MF C30 H62 N4 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Currently available stereo shown.



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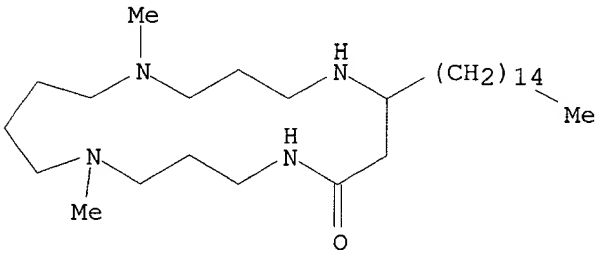
L11 ANSWER 9 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 178494-84-3 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 1,13-dimethyl-8-pentadecyl-, (-)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **5-Normethylbudmunchiamine K**
FS STEREOSEARCH
MF C30 H62 N4 O
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Rotation (-).
Currently available stereo shown.



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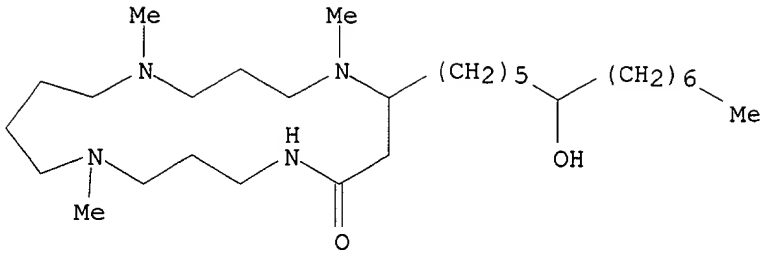
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L11 ANSWER 10 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 178494-83-2 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 8-(6-hydroxytridecyl)-1,9,13-trimethyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **6'.xi.-Hydroxybudmunchiamine C**
MF C29 H60 N4 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Currently available stereo shown.



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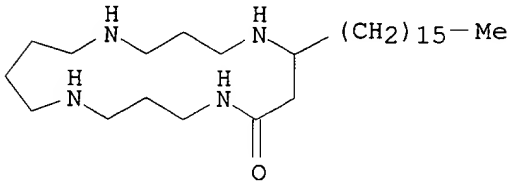
2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L11 ANSWER 11 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 165561-01-3 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 8-hexadecyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine L 1**
MF C29 H60 N4 O
SR CA
LC STN Files: CA, CAPLUS



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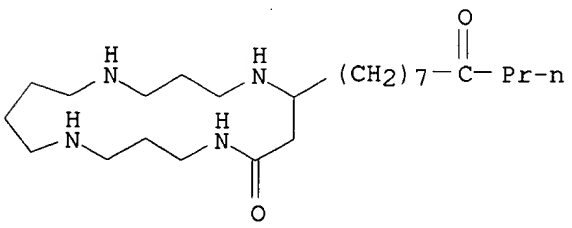
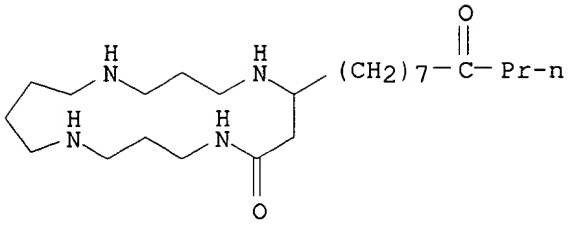
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L11 ANSWER 12 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 165467-48-1 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 8-(8-oxoundecyl)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine L 3**
MF C24 H48 N4 O2
SR CA
LC STN Files: CA, CAPLUS

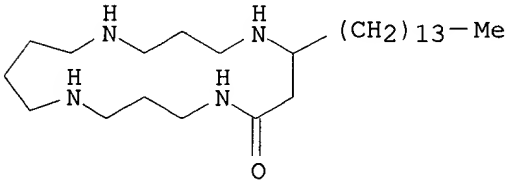




PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

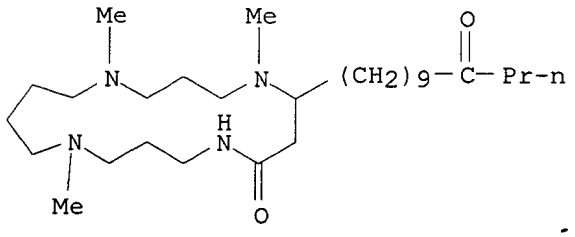
L11 ANSWER 13 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 165467-47-0 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 8-tetradecyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine L 2**
MF C27 H56 N4 O
SR CA
LC STN Files: CA, CAPLUS

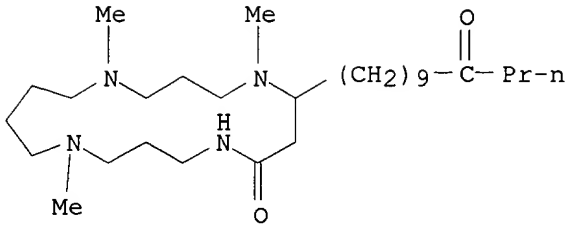


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L11 ANSWER 14 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 143070-37-5 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 1,9,13-trimethyl-8-(10-oxotridecyl)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine D**
MF C29 H58 N4 O2
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

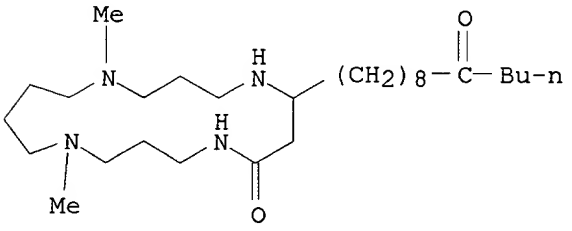




PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

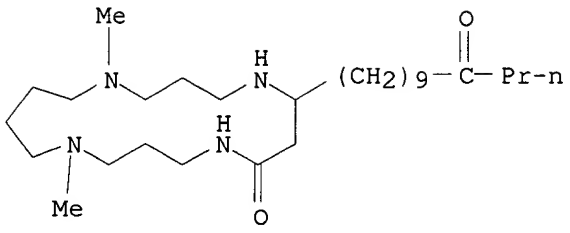
L11 ANSWER 15 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 143051-90-5 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 1,13-dimethyl-8-(9-oxotridecyl)-(9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine I**
MF C28 H56 N4 O2
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

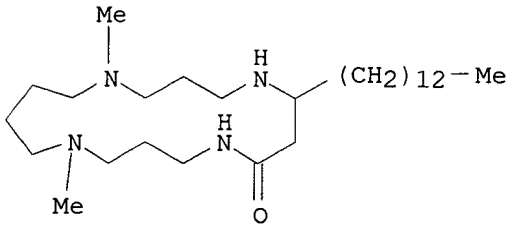
L11 ANSWER 16 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 143051-89-2 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 1,13-dimethyl-8-(10-oxododecyl)-(9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine H**
MF C28 H56 N4 O2
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

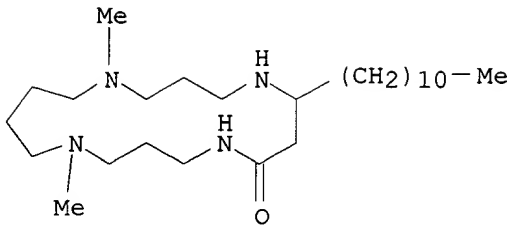
L11 ANSWER 17 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 143051-88-1 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 1,13-dimethyl-8-tridecyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine G**
MF C28 H58 N4 O
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

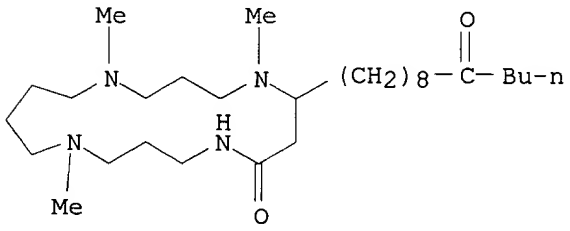
L11 ANSWER 18 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 143051-87-0 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 1,13-dimethyl-8-undecyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine F**
MF C26 H54 N4 O
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

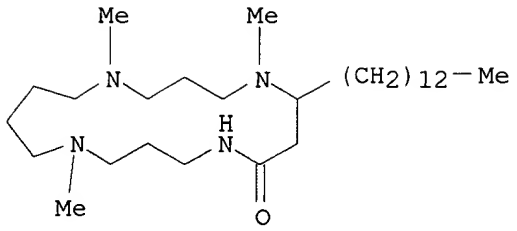
L11 ANSWER 19 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 143051-86-9 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 1,9,13-trimethyl-8-(9-oxotridecyl)-(9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine E**
MF C29 H58 N4 O2
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

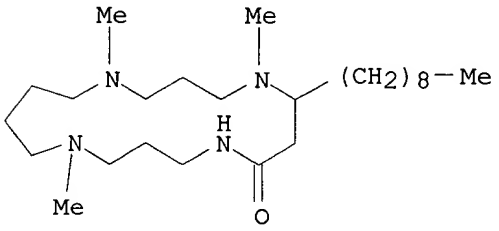
L11 ANSWER 20 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 139750-78-0 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 1,9,13-trimethyl-8-tridecyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine C**
MF C29 H60 N4 O
SR CA
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAPLUS, CASREACT, TOXCENTER
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1962 TO DATE)
4 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L11 ANSWER 21 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 139750-77-9 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 1,9,13-trimethyl-8-nonyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine B**
MF C25 H52 N4 O
SR CA
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAPLUS, CASREACT, TOXCENTER
(*File contains numerically searchable property data)

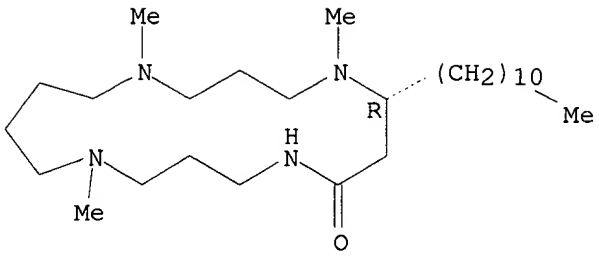


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1962 TO DATE)
4 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L11 ANSWER 22 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 139750-76-8 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 1,9,13-trimethyl-8-undecyl-, (8R)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **(-)-(R)-Budmunchiamine A**
CN **Budmunchiamine A**
FS STEREOSEARCH
MF C27 H56 N4 O
SR CA
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

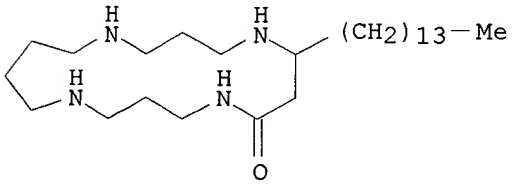
10 REFERENCES IN FILE CA (1962 TO DATE)
10 REFERENCES IN FILE CAPLUS (1962 TO DATE)

=> d l11 13 all

L11 ANSWER 13 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 165467-47-0 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 8-tetradecyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Budmunchiamine L 2**
MF C27 H56 N4 O
SR CA
LC STN Files: CA, CAPLUS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C13N4	NC3NC3NC3NC4	17	C13N4	4584.21.2	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1	pH 1	(1) ACD
Bioconc. Factor (BCF)	1	pH 4	(1) ACD
Bioconc. Factor (BCF)	1	pH 7	(1) ACD
Bioconc. Factor (BCF)	1	pH 8	(1) ACD
Bioconc. Factor (BCF)	1893	pH 10	(1) ACD

Boiling Point (BP)	611.2+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	90.76+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	132.6+/-57.0 deg C		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	4		(1) ACD
Koc (KOC)	1	pH 1	(1) ACD
Koc (KOC)	1	pH 4	(1) ACD
Koc (KOC)	1	pH 7	(1) ACD
Koc (KOC)	1	pH 8	(1) ACD
Koc (KOC)	2878	pH 10	(1) ACD
logD (LOGD)	0.59	pH 1	(1) ACD
logD (LOGD)	0.60	pH 4	(1) ACD
logD (LOGD)	0.63	pH 7	(1) ACD
logD (LOGD)	1.01	pH 8	(1) ACD
logD (LOGD)	5.09	pH 10	(1) ACD
logP (LOGP)	6.598+/-0.417		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	452.76		(1) ACD
pKa (PKA)	10.79+/-0.40	Most Basic	(1) ACD
Vapor Pressure (VP)	7.02E-15 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1

AN 123:79654 CA
TI N-Demethyl budmunchiamines from Albizzia lebbek seeds
AU Misra, Laxmi N.; Dixit, Ajay K.; Wagner, Hildebert
CS Phytochem. Technol. Div., Cent. Inst. Med. Aromatic Plants, Lucknow, 226015, India
SO Phytochemistry (1995), 39(1), 247-9
CODEN: PYTCAS; ISSN: 0031-9422
PB Elsevier
DT Journal
LA English
CC 11-1 (Plant Biochemistry)
Section cross-reference(s): 31
AB A methanol ext. of the seeds of Albizzia lebbek has yielded three new macrocyclic spermine alkaloids, budmunchiamines L1-L3. The structures have been detd. by spectral anal., chem. transformations and comparison with budmunchiamines A-I.
ST budmunchiamine alkaloid Albizzia
IT Albizia lebbek
(N-demethyl budmunchiamines from Albizzia lebbek seeds)
IT Nomenclature, new natural products
(budmunchiamine L-1 (alkaloid))
IT Nomenclature, new natural products
(budmunchiamine L-2 (alkaloid))
IT Nomenclature, new natural products
(budmunchiamine L-3 (alkaloid))
IT Molecular structure, natural product
(of budmunchiamine L-1 (alkaloid))
IT Molecular structure, natural product
(of budmunchiamine L-2 (alkaloid))

IT Molecular structure, natural product
(of budmunchiamine L-3 (alkaloid))
IT Alkaloids, biological studies
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(spermine; N-demethyl budmunchiamines from Albizzia lebbek seeds)
IT 165467-47-0P, Budmunchiamine L 2 165467-48-1P, Budmunchiamine L 3
165561-01-3P, Budmunchiamine L 1
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(N-demethyl budmunchiamines from Albizzia lebbek seeds)
IT 164933-35-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

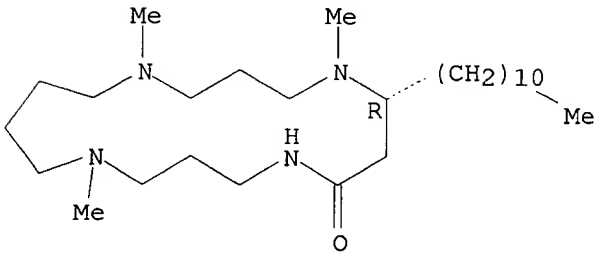
=> d l11 22 all

L11 ANSWER 22 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN 139750-76-8 REGISTRY
CN 1,5,9,13-Tetraazacycloheptadecan-6-one, 1,9,13-trimethyl-8-undecyl-, (8R)-(9CI) (CA INDEX NAME)
OTHER NAMES:
CN **(-)-(R)-Budmunchiamine A**
CN **Budmunchiamine A**
FS STEREOSEARCH
MF C27 H56 N4 O
SR CA
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C13N4	NC3NC3NC3NC4	17	C13N4	4584.21.2	1

Absolute stereochemistry. Rotation (-).



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1	pH 1	(1) ACD
Bioconc. Factor (BCF)	1	pH 4	(1) ACD
Bioconc. Factor (BCF)	1	pH 7	(1) ACD
Bioconc. Factor (BCF)	17.6	pH 8	(1) ACD
Bioconc. Factor (BCF)	16748	pH 10	(1) ACD
Boiling Point (BP)	570.3+/-50.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	85.54+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	298.7+/-54.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	10		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	1		(1) ACD
Koc (KOC)	1	pH 1	(1) ACD
Koc (KOC)	1	pH 4	(1) ACD
Koc (KOC)	1	pH 7	(1) ACD
Koc (KOC)	32.8	pH 8	(1) ACD
Koc (KOC)	31335	pH 10	(1) ACD
logD (LOGD)	0.17	pH 1	(1) ACD
logD (LOGD)	0.18	pH 4	(1) ACD
logD (LOGD)	0.68	pH 7	(1) ACD
logD (LOGD)	2.96	pH 8	(1) ACD
logD (LOGD)	5.94	pH 10	(1) ACD
logP (LOGP)	6.180+/-0.431		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	452.76		(1) ACD
pKa (PKA)	9.54+/-0.70	Most Basic	(1) ACD
Vapor Pressure (VP)	5.10E-13 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD)

10 REFERENCES IN FILE CA (1962 TO DATE)
10 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1

AN 137:295138 CA
TI (-)-(3S)-3-(Tosylamino)butano-4-lactone, a versatile chiral synthon for the enantioselective synthesis of different types of polyamine macrocycles: determination of the absolute configuration of (-)-(R)-budmunchiamine A
AU Detterbeck, Richard; Guggisberg, Armin; Popaj, Kasim; Hesse, Manfred
CS Organisch-chemisches Institut der Universitat Zurich, Zurich, CH-8057, Switz.
SO Helvetica Chimica Acta (2002), 85(6), 1742-1758
CODEN: HCACAV; ISSN: 0018-019X
PB Verlag Helvetica Chimica Acta
DT Journal
LA English
CC 31-6 (Alkaloids)
AB (-)-(3S)-3-(Tosylamino)butano-4-lactone and its deriv. Et (-)-(3S)-4-iodo-3-(tosylamino)butanoate are presented as easily accessible chiral building blocks for the construction of a range of different macrolactam frameworks important for the synthesis of naturally occurring polyamine alkaloids as well as for establishing a substance library of

such compds., including S-contg. derivs. for biol. tests. In addn. to that, the abs. configuration of the spermine alkaloid (-)-(R)-budmunchiamine A from Albizia amara was detd. by total synthesis according to the new methodol.

ST budmunchiamine A prepn abs configuration; tosylaminobutanolactone chiral synthon polyamine macrocycle; enantioselective synthesis polyamine macrocycle tosylaminobutanolactone chiral synthon; butanolactone tosylamino chiral synthon enantioselective synthesis polyamine macrocycle; lactone butano tosylamino chiral synthon enantioselective synthesis polyamine macrocycle

IT Crystal structure
Molecular structure
(of heptenyltosyltriazacyclotriedecanone)

IT Absolute configuration
Asymmetric synthesis and induction
(use of (tosylamino)butano-4-lactones as chiral synthons in asym. synthesis of polyamine macrocycles and budmunchiamine A and abs. configuration of (-)-(R)-budmunchiamine A)

IT 139750-76-8P, (-)-(R)-Budmunchiamine A
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(use of (tosylamino)butano-4-lactones as chiral synthons in asym. synthesis of polyamine macrocycles and budmunchiamine A and abs. configuration of (-)-(R)-budmunchiamine A)

IT 107-13-1, Acrylonitrile, reactions 109-64-8, 1,3-Dibromopropane 109-76-2, Propane-1,3-diamine 110-60-1, 1,4-Butanediamine 111-88-6, Octane-1-thiol 928-96-1, (Z)-Hex-3-en-1-ol 2050-77-3, 1-Iododecane 4724-56-5, Butane-1,4-diol bis(4-methylbenzenesulfonate) 5469-66-9, Propane-1,3-diol bis(4-methylbenzenesulfonate) 147228-21-5 147228-22-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(use of (tosylamino)butano-4-lactones as chiral synthons in asym. synthesis of polyamine macrocycles and budmunchiamine A and abs. configuration of (-)-(R)-budmunchiamine A)

IT 4748-73-6P 21676-03-9P, (Z)-1-Iodohex-3-ene 91652-58-3P 96624-91-8P 150059-33-9P 467457-05-2P 467457-07-4P 467457-08-5P 467457-13-2P 467457-16-5P 467457-17-6P 467457-19-8P 467457-28-9P 467457-36-9P 467457-38-1P 467457-40-5P 467457-42-7P 467457-49-4P 467457-51-8P 467457-53-0P 467457-55-2P 467457-57-4P 467457-59-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(use of (tosylamino)butano-4-lactones as chiral synthons in asym. synthesis of polyamine macrocycles and budmunchiamine A and abs. configuration of (-)-(R)-budmunchiamine A)

IT 467457-10-9P 467457-20-1P 467457-22-3P 467457-31-4P 467457-44-9P 467457-46-1P 467457-61-0P 467457-63-2P 467457-64-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(use of (tosylamino)butano-4-lactones as chiral synthons in asym. synthesis of polyamine macrocycles and budmunchiamine A and abs. configuration of (-)-(R)-budmunchiamine A)

IT 467457-09-6P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(use of (tosylamino)butano-4-lactones as chiral synthons in asym. synthesis of polyamine macrocycles and budmunchiamine A and abs. configuration of (-)-(R)-budmunchiamine A and crystal structure of heptenyltriazacyclotridecanone deriv.)

RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD

(1) Altomare, A; J Appl Crystallogr 1994, P435
(2) Bergmeier, S; J Org Chem 1993, V58, P5019 CAPLUS
(3) Bernardinelli, G; Acta Crystallogr, Sect A 1985, V41, P500
(4) Chavez, F; J Org Chem 1989, V54, P2990 CAPLUS
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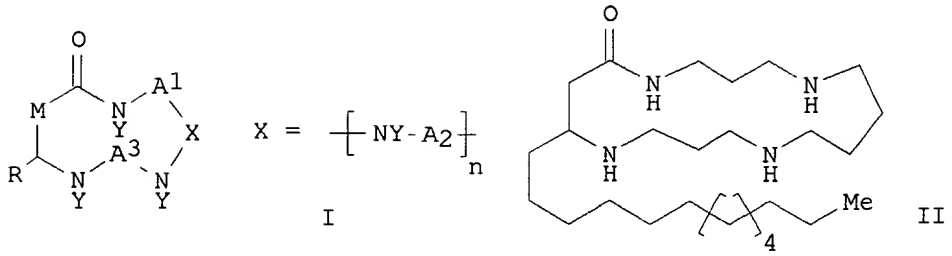
REFERENCE 2

AN 136:167548 CA
TI Synthesis of cyclic polyamine analogs for cancer therapy
IN Frydman, Benjamin; Hesse, Manfred; Guggisberg, Armin; Popaj, Kasmin; Drandarov, Konstantin; Basu, Hirak; Bhattacharya, Subhra; Wang, Yu
PA Slil Biomedical Corporation, USA
SO PCT Int. Appl., 105 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D257-02
ICS C07D255-02; A61K031-395; A61P035-00
CC 31-6 (Alkaloids)
Section cross-reference(s): 1
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002010142	A1	20020207	WO 2001-US24282	20010802

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2000-222522P 20000802
GI



I II

AB Novel cyclic polyamine compds., such as I [A1, A2 = C1-C8 alkyl; Y = H, C1-C4 alkyl; M = C1-C4 alkyl; n = 0-3; R = C1-C32 alkyl], as well as all stereoisomers and salts thereof, were prepd. for treating diseases caused by uncontrolled proliferation of cells, such as cancer, esp. prostate cancer, and for inducing intracellular ATP hydrolysis for treatment of other disorders. Thus, cyclic polyamine II was prepd. via multistep synthetic sequence starting from triphenylphosphine, Et bromoacetate, myristylaldehyde and spermine. II.3HCl showed ID50 = 0.83.mu.M on prostate tumor cell growth.

ST polyamine cyclic prepn anticancer budmunchiamine

IT Polyamines
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(analog; prepn. of cyclic polyamine analogs for cancer therapy)

IT Cyclization
(lactamization, macrolactamization; in prepn. of cyclic polyamine analogs for cancer therapy)

IT Macrocyclization
(macrolactamization; in prepn. of cyclic polyamine analogs for cancer therapy)

IT Prostate gland
(neoplasm, inhibitors; prepn. of cyclic polyamine analogs for cancer therapy)

IT Cytotoxicity
(of cyclic polyamine analogs on survival of DuPro cells)

IT Alkylation
(of secondary amino groups in prepn. of cyclic polyamine analogs for cancer therapy)

IT Peptides, biological studies
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pentapeptides; prepn. of cyclic polyamine analogs for cancer therapy)

IT Antitumor agents
(prostate gland; prepn. of cyclic polyamine analogs for cancer therapy)

IT Peptides, biological studies
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(tetrapeptides; prepn. of cyclic polyamine analogs for cancer therapy)

IT 56-65-5, ATP, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(hydrolysis; in a cancerous cell via cyclic polyamine analogs)

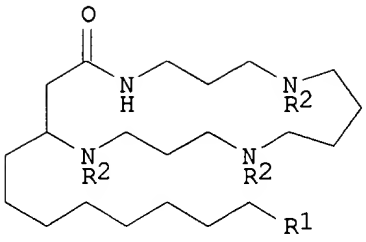
IT 4375-83-1, Tris(dimethylamino)borane
RL: RGT (Reagent); RACT (Reactant or reagent)
(in prepn. of cyclic polyamine analogs for cancer therapy)

IT 139750-76-8P 139750-77-9P 396117-44-5P, SL 11239 396117-45-6P, SL 11238 396117-46-7P, SL 11174 396117-47-8P, SL 11197 396117-48-9P, SL 11199 396117-49-0P, SL 11200 396117-50-3P, SL 11208
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of cyclic polyamine analogs for cancer therapy)

IT 395649-52-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of cyclic polyamine analogs for cancer therapy)
IT 110-60-1P, Putrescine 124-20-9P, Spermidine
RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of cyclic polyamine analogs for cancer therapy)
IT 50-00-0, Formalin, reactions 71-44-3, Spermine 105-36-2, Ethyl bromoacetate 107-13-1, Acrylonitrile, reactions 112-31-2, Caprinaldehyde 112-54-9, Laurinaldehyde 124-25-4, Myristinaldehyde 603-35-0, Triphenylphosphine, reactions 73453-98-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of cyclic polyamine analogs for cancer therapy)
IT 1530-45-6P 28290-90-6P 38112-60-6P 42778-95-0P 75814-58-3P 135251-95-5P 139750-78-0P, Budmunchiamine C 335153-35-0P 335153-39-4P 335153-41-8P 335153-43-0P 395649-49-7P 395649-50-0P 395649-51-1P 395649-53-3P 395649-54-4P 395649-55-5P 395649-56-6P 395649-57-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of cyclic polyamine analogs for cancer therapy)
IT 10433-06-4, Antimony(III)ethoxide 25895-60-7, Sodium cyanoborohydride
RL: RGT (Reagent); RACT (Reactant or reagent)
(prepn. of cyclic polyamine analogs for cancer therapy)
RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Squibb Bristol Myers Co; EP 0451547 A 1991 CAPLUS
(2) Univ Hawaii; EP 0792875 A 1997 CAPLUS

REFERENCE 3

AN 134:311341 CA
TI Syntheses of macrocyclic spermine alkaloids (.+-.)-budmunchiamine A-C
AU Popaj, Kasim; Hesse, Manfred
CS Organisch-chemisches Institut der Universitat Zurich, Zurich, CH-8057, Switz.
SO Helvetica Chimica Acta (2001), 84(1), 180-186
CODEN: HCACAV; ISSN: 0018-019X
PB Verlag Helvetica Chimica Acta
DT Journal
LA English
CC 31-6 (Alkaloids)
GI



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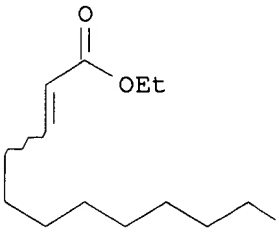

II

AB The syntheses of four macrocyclic spermine alkaloids, (.+-.)-budmunchiamine A-C (I, R1 = Pr, Me, pentyl; R2 = Me) and (.+-.)-budmunchiamine L4, (I, R1 = CH2(CH2)11Me, R2 = H) were accomplished by Michael addn. of spermine to the .alpha.,.beta.-unsatd. esters II, followed by cyclization of the resulting .alpha.,.omega.-tetraamino esters with triethoxyantimony; N-methylation of the amino lactams yielded the budmunchiamines A-C.

ST budmunchiamine macrocyclic spermine alkaloid synthesis; Michael addn budmunchiamine macrocyclic spermine alkaloid synthesis

IT Alkaloids, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(macrocyclic spermine; syntheses (.+-.)-budmunchiamine A-C)

IT Michael reaction
(syntheses of macrocyclic spermine alkaloids (.+-.)-budmunchiamine A-C)

IT 71-44-3, Spermine 105-36-2 112-31-2, Decanal 112-54-9, Dodecanal 124-25-4, Tetradecanal 661-19-8, Docosan-1-ol
RL: RCT (Reactant); RACT (Reactant or reagent)
(syntheses of macrocyclic spermine alkaloids (.+-.)-budmunchiamine A-C)

IT 1530-45-6P 57402-36-5P, Docosanal 61621-59-8P 78217-11-5P 335153-25-8P 335153-29-2P 335153-31-6P 335153-33-8P 335153-35-0P 335153-37-2P 335153-39-4P 335153-41-8P 335153-43-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(syntheses of macrocyclic spermine alkaloids (.+-.)-budmunchiamine A-C)

IT 139750-76-8P, Budmunchiamine A 139750-77-9P, Budmunchiamine B 139750-78-0P, Budmunchiamine C 335153-45-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(syntheses of macrocyclic spermine alkaloids (.+-.)-budmunchiamine A-C)

RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
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(2) Corey, E; Tetrahedron Lett 1975, V31, P2647
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(9) Pezzuto, J; Phytochemistry 1992, V32, P1795
(10) Rukunga, G; J Nat Prod 1996, V59, P850 CAPLUS

(11) Rukunga, G; Phytochemistry 1996, V42, P1211 CAPLUS
(12) Wiesner, K; Can J Chem 1952, V30, P761
(13) Wiesner, K; Can J Chem 1968, V46, P1881 CAPLUS
(14) Wiesner, K; Can J Chem 1968, V46, P3617 CAPLUS

REFERENCE 4

AN 132:203164 CA
TI Calcium receptor-active molecules
IN Nemeth, Edward F.; Van Wanegen, Bradford C.; Balandrin, Manuel F.; Delmar, Eric M.; Moe, Scott T.
PA NPS Pharmaceuticals, Inc., USA
SO U.S., 194 pp., Cont.-in-part of U.S. Ser. No. 353,784.
CODEN: USXXAM
DT Patent
LA English
IC A61K031-44; A61K311-35; A01N033-02; A01N037-18
NCL 514579000
CC 1-12 (Pharmacology)
Section cross-reference(s): 3, 15, 25
FAN.CNT 9

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6031003	A	20000229	US 1995-484719	19950607
	JP 09281209	A2	19971031	JP 1996-232165	19920821
	JP 09328420	A2	19971222	JP 1996-232130	19920821
	JP 11221095	A2	19990817	JP 1998-313631	19920821
	JP 3256502	B2	20020212		
	JP 2001220356	A2	20010814	JP 2000-394979	19920821
	EP 1281702	A2	20030205	EP 2002-16612	19920821
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, IE				
	CN 1071333	A	19930428	CN 1992-111580	19920822
	CN 1067550	B	20010627		
	IL 102917	A1	20001206	IL 1992-102917	19920823
	ZA 9206360	A	19930330	ZA 1992-6360	19920824
	CA 2173747	AA	19950427	CA 1994-2173747	19941021
	WO 9511221	A1	19950427	WO 1994-US12117	19941021
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, US				
	RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9480872	A1	19950508	AU 1994-80872	19941021
	AU 702629	B2	19990225		
	EP 724561	A1	19960807	EP 1994-931982	19941021
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	CN 1139917	A	19970108	CN 1994-194577	19941021
	JP 09504032	T2	19970422	JP 1994-512244	19941021
	US 6011068	A	20000104	US 1994-353784	19941208
	AU 9671977	A1	19970220	AU 1996-71977	19961125
	AU 711247	B2	19991007		
	AU 9931226	A1	19990722	AU 1999-31226	19990524
	AU 747853	B2	20020523	AU 1999-61707	19991126
	AU 9961707	A1	20000224		

PRAI	US 1991-749451	19910823
	US 1992-834044	19920211
	US 1992-934161	19920821
	US 1993-17127	19930212
	US 1993-9389	19930223
	US 1993-141248	19931022

US 1994-292827 19940819
WO 1994-US12117 19941021
US 1994-353784 19941208
EP 1992-919933 19920821
JP 1992-504650 19920821
JP 1996-232165 19920821
JP 1998-313631 19920821
AU 1994-80872 19941021

AB The present invention relates to the different roles inorg. ion receptors have in cellular and body processes. The present invention features: (1) mols. which can modulate one or more inorg. ion receptor activities, preferably the mol. can mimic or block an effect of an extracellular ion on a cell having an inorg. ion receptor, more preferably the extracellular ion is Ca2 and the effect is on a cell having a calcium receptor; (2) inorg. ion receptor proteins and fragments thereof, preferably calcium receptor proteins and fragments thereof; (3) nucleic acids encoding inorg. ion receptor proteins and fragments thereof, preferably calcium receptor proteins and fragments thereof; (4) antibodies and fragments thereof, targeted to inorg. ion receptor proteins, preferably calcium receptor protein; and (5) uses of such mols., proteins, nucleic acids and antibodies. For example, NPS R-568 ((R)-(+)-N-[3-(2-chlorophenyl)propyl]-.alpha.-methyl-3-methoxybenzylamine) was synthesized and its effectiveness was evaluated in a placebo-controlled, single-dose, dose-escalation format in a healthy, post-menopausal women. NPS R-568 caused a transient dose-dependent decrease in plasma PTH concn., and , at higher doses, a decrease in serum ionized serum concn. in the human subject. There was no apparent change in serum calcitonin at the doses studied. Higher doses are expected to affect calcitonin levels as obsd. in rats.

ST calcimimetic calcilytic calcium receptor antiosteoporotic; fendiline analog calcium receptor modulator antiosteoporotic; antibody polyamine calcium receptor modulator

IT Animal cell line
(Hek 293; screening of calcium receptor-active mols. for treatment of osteoporosis and related disorders)

IT Bone, disease
(Paget's; prepn. of calcium receptor-active mols. for treatment of osteoporosis and related disorders)

IT Antibodies
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); MFM (Metabolic formation); THU (Therapeutic use); BIOL (Biological study); FORM (Formation, nonpreparative); USES (Uses)
(against calcium receptors; prepn. of calcium receptor-active mols. for treatment of osteoporosis and related disorders)

IT Diagnosis
(agents; prepn. of calcium receptor-active mols. for treatment of osteoporosis and related disorders)

IT Antibiotics
(aminoglycoside; prepn. of calcium receptor-active mols. for treatment of osteoporosis and related disorders)

IT Receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(calcium; calcium receptor-active mols. for treatment of osteoporosis and related disorders)

IT Amines, biological studies
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(cyclic, polyamines; prepn. of calcium receptor-active mols. for treatment of osteoporosis and related disorders)

IT Egg
(oocyte; screening of calcium receptor-active mols. for treatment of

osteoporosis and related disorders)

IT Amines, biological studies
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(polyamines, nonpolymeric; prepn. of calcium receptor-active mols. for treatment of osteoporosis and related disorders)

IT DNA sequences
Protein sequences
(prepn. and screening of calcium receptor-active mols. for treatment of osteoporosis and related disorders)

IT Gene therapy
Hyperparathyroidism
(prepn. of calcium receptor-active mols. for treatment of osteoporosis and related disorders)

IT Antisense oligonucleotides
Protamines
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(prepn. of calcium receptor-active mols. for treatment of osteoporosis and related disorders)

IT Bone
(resorption, inhibitors; calcium receptor-active mols. for treatment of osteoporosis and related disorders)

IT Drug screening
Osteoclast
Parathyroid gland
(screening of calcium receptor-active mols. for treatment of osteoporosis and related disorders)

IT Osteoporosis
(therapeutic agents; calcium receptor-active mols. for treatment of osteoporosis and related disorders)

IT 219686-09-6 219686-11-0 219686-12-1 219686-13-2 219686-14-3 219686-15-4 219686-16-5
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); OCCU (Occurrence)
(antibodies against; prepn. and screening of calcium receptor-active mols. for treatment of osteoporosis and related disorders)

IT 52-53-9, Verapamil 57-92-1, Streptomycin, biological studies 71-44-3, Spermine 112-24-3, Triethylenetetramine 112-57-2, Tetraethylenepentamine 119-04-0, Neomycin B 124-20-9, Spermidine 296-35-5, Hexacyclen 1403-66-3, Gentamicin 2783-17-7, 1,12-Diaminododecane 4067-16-7, Pentaethylenehexamine 4696-76-8, Bekanamycin 13042-18-7, Fendiline 16662-47-8 21829-25-4, Nifedipine 24937-47-1, Polyarginine, SRU 25104-18-1, Polylysine 25212-18-4, Polyarginine 25876-10-2, Gentamicin C1 25876-11-3, Gentamicin C2 26098-04-4, Gentamicin C1a 38000-06-5 39562-70-4, Nitrendipine 42399-41-7, Diltiazem 57818-92-5, TMB-8 71145-03-4, Bay K 8644 78005-41-1, Protamine CII (Oncorhynchus mykiss testis) 85610-72-6, (R)-Prenylamine 87955-89-3, NPS 383 97217-83-9, (+)-202-791 97217-84-0, (-)-202-791 105029-41-2, Argiotoxin 636 108393-62-0, (R)-Fendiline 108448-58-4, (S)-Fendiline 111944-83-3, Argiotoxin 659 115976-91-5, Philanthotoxin 433 128549-96-2, AGA 489 128549-97-3, AGA 505 133805-32-0, NPS 019 139750-76-8, Budmunchiamine A 148717-51-5, NPS 382 148717-52-6, NPS 384 148740-50-5, NPS 381 148740-51-6, NPS 021 148740-52-7, NPS S-467 159149-75-4, NPS S-568 199614-43-2 199614-44-3
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(calcium receptor-active mols. for treatment of osteoporosis and related disorders)

IT 7440-70-2, Calcium, biological studies 9002-64-6, Parathyroid hormone 9007-12-9, Calcitonin
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(calcium receptor-active mols. for treatment of osteoporosis and related disorders)

IT 153834-08-3 161663-06-5 168183-63-9 168257-64-5 206370-64-1, 10: PN: US6011068 SEQID: 1 unclaimed DNA 206370-65-2 206370-66-3 206370-67-4 206370-68-5 206370-69-6 206370-70-9, GenBank I75057 206370-71-0, GenBank I75058 219686-07-4
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); OCCU (Occurrence)
(prepn. and screening of calcium receptor-active mols. for treatment of osteoporosis and related disorders)

IT 66469-40-7P 148717-47-9P, NPS 467 148717-48-0P 148717-49-1P, NPS 568 148717-54-8P, NPS R-568 148717-56-0P, NPS R-467 159149-76-5P 159149-96-9P 159149-97-0P 159149-98-1P 159149-99-2P 159150-00-2P 159150-03-5P 159150-04-6P 159150-05-7P 159150-06-8P 159150-17-1P 159150-18-2P 159150-19-3P 159150-20-6P 159150-28-4P 159150-29-5P 159247-74-2P 165304-87-0P 179381-56-7P 179381-60-3P 179381-62-5P 179381-67-0P 179381-69-2P 179381-70-5P 179381-74-9P 179381-75-0P 179603-34-0P 179603-36-2P 179603-37-3P 179603-38-4P 179603-40-8P 179603-41-9P 179603-42-0P 199614-53-4P 199614-61-4P 199614-63-6P 199614-68-1P 199614-73-8P 199614-84-1P 199614-85-2P 199614-86-3P 199614-87-4P 199614-89-6P 199614-90-9P 199614-91-0P 199614-93-2P 199614-94-3P 199614-95-4P 199614-97-6P 199614-98-7P 199614-99-8P 199615-00-4P 199615-01-5P 199615-02-6P 199615-03-7P 199615-05-9P 199615-06-0P 199615-07-1P 199615-08-2P 199615-09-3P 199615-11-7P 199615-13-9P 199615-14-0P 199615-15-1P 199615-16-2P 199615-17-3P 199615-18-4P 199615-22-0P 199615-23-1P 199615-25-3P 199615-26-4P 199615-27-5P 199615-28-6P 199615-29-7P 219686-00-7P 219686-01-8P 226256-47-9P 252055-76-8P 252055-78-0P 252055-80-4P 252055-81-5P 252055-83-7P 252055-88-2P 252056-03-4P 252056-10-3P 253337-19-8P 253337-22-3P 253337-23-4P 253337-24-5P 253337-26-7P 253337-27-8P 253337-28-9P 253337-29-0P 253337-30-3P 253337-32-5P 253337-33-6P 253337-34-7P 253337-35-8P 253337-36-9P 253337-39-2P 253337-41-6P 253337-42-7P 253337-43-8P 253337-44-9P 253337-45-0P 253337-46-1P 253337-47-2P 253337-49-4P 253337-50-7P 253337-51-8P 253337-52-9P 253337-53-0P 253337-54-1P 253337-55-2P 253337-56-3P 253337-57-4P 253337-58-5P 253337-59-6P 253337-60-9P 253337-61-0P 253337-62-1P 253337-63-2P 253337-64-3P 253337-65-4P 253337-66-5P 259855-78-2P 259855-79-3P 259855-80-6P 259855-81-7P 259855-83-9P 259855-84-0P 259855-85-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of calcium receptor-active mols. for treatment of osteoporosis and related disorders)

IT 199615-10-6 199615-19-5
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(prepn. of calcium receptor-active mols. for treatment of osteoporosis and related disorders)

IT 93-08-3, 2'-Acetonaphthone 99-03-6, 3'-Aminoacetophenone 100-06-1, 4'-Methoxyacetophenone 122-03-2, 4-Isopropylbenzaldehyde 586-37-8, 3'-Methoxyacetophenone 876-02-8, 4'-Hydroxy-3'-methylacetophenone 941-98-0, 1'-Acetonaphthone 1504-74-1, 2-Methoxycinnamaldehyde 2038-57-5, 3-Phenylpropylamine 2420-16-8, 3-Chloro-4-hydroxybenzaldehyde 3886-70-2 4903-09-7, 3-Chloro-4-methoxybenzaldehyde 7315-17-5,

2-Chlorohydrocinnamonitrile 18655-48-6 68376-32-9,
2-Methylcinnamonitrile 88196-70-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of calcium receptor-active mols. for treatment of osteoporosis and related disorders)

IT 1441-99-2P, 3'-Thiomethylacetophenone 10024-90-5P 37612-52-5P 124829-13-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of calcium receptor-active mols. for treatment of osteoporosis and related disorders)

IT 179381-55-6P 179381-59-0P 179381-63-6P 179381-65-8P 179381-66-9P 252055-41-7P 259855-86-2P 259855-87-3P 259855-88-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of calcium receptor-active mols. for treatment of osteoporosis and related disorders)

RE.CNT 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD

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(25) Fujino; US 3972859 1976 CAPLUS
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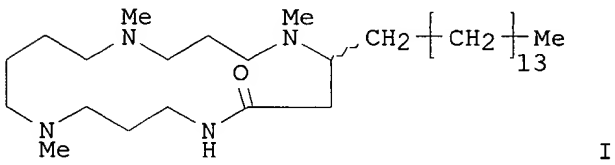
REFERENCE 5

AN 125:163232 CA
TI New macrocyclic spermine (budmunchiamine) alkaloids from Albizia gummifera: with some observations on the structure-activity relationships of the budmunchiamines
AU Rukunga, Geoffrey M.; Waterman, Peter G.
CS Department of Pharmaceutical Sciences, University of Strathclyde, Glasgow, G1 1XW, UK
SO Journal of Natural Products (1996), 59(9), 850-853
CODEN: JNPRDF; ISSN: 0163-3864
PB American Chemical Society
DT Journal
LA English
CC 11-1 (Plant Biochemistry)
Section cross-reference(s): 1, 31
GI



I

AB The CH2Cl2 ext. of the stem bark of Albizia gummifera yielded four macrocyclic spermine alkaloids (budmunchiamines), three of them being new analogs. On the basis of spectral anal. and comparison with related compds. they were identified as budmunchiamine G and the new analogs budmunchiamine K (I), 6'.xi.-hydroxybudmunchiamine K , and 9-normethylbudmunchiamine K. The four isolated alkaloids and other related budmunchiamines isolated from Albizia schimperana were all active against two Gram-pos. and two Gram-neg. bacteria at MIC levels below 80 .mu.g mL-1, and showed toxicity to brine shrimp larvae (with LC50 values below 100 .mu.g mL-1). The neg. impact of side chain hydroxylation and N-demethylation on both measures of biol. activity was shown to be considerable.
ST Albizia alkaloid budmunchiamine antibacterial cytotoxicity structure
IT Albizia gummifera
(antibacterial and cytotoxic spermine alkaloids from)
IT Alkaloids, biological studies
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(antibacterial and cytotoxic spermine alkaloids from Albizia gummifera)
IT Nomenclature, new natural products
(budmunchiamine K (spermine alkaloid))
IT Bactericides, Disinfectants, and Antiseptics
Cytotoxic agents
(budmunchiamine spermine alkaloids from Albizia gummifera as)
IT Molecular structure, natural product

(of budmunchiamine K (spermine alkaloid))
IT Molecular structure-biological activity relationship
(bactericidal, of budmunchiamine spermine alkaloids from Albizia)
IT 139750-76-8, Budmunchiamine A 178494-83-2, 6'.xi.-Hydroxybudmunchiamine C 178494-84-3, 5-Normethylbudmunchiamine K 178494-85-4, 6'.xi.-Hydroxy-5-normethylbudmunchiamine K 178494-86-5, 14-Normethylbudmunchiamine K
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(antibacterial and cytotoxic activity of)
IT 143051-88-1, Budmunchiamine G
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(antibacterial and cytotoxic spermine alkaloids from Albizia gummifera)
IT 178494-87-6P, Budmunchiamine K 180285-72-7P, 6'.xi.-Hydroxybudmunchiamine K 180285-78-3P, 9-Normethylbudmunchiamine K
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(antibacterial and cytotoxic spermine alkaloids from Albizia gummifera)

REFERENCE 6

AN 125:81874 CA
TI Spermine alkaloids from Albizia schimperiana
AU Rukunga, Geoffrey A.; Waterman, Peter G.
CS Phytochem. Res. Lab., Univ. Strathclyde, Glasgow, GI IXW, UK
SO Phytochemistry (1996), 42(4), 1211-1215
CODEN: PYTCAS; ISSN: 0031-9422
PB Elsevier
DT Journal
LA English
CC 11-1 (Plant Biochemistry)
Section cross-reference(s): 31
AB The dichloromethane ext. of the stem bark of A. schimperiana yielded 5 macrocyclic spermine alkaloids (budmunchiamies), 4 of them novel. The structures of these compd. were elucidated by spectral anal. and comparison with literature.
ST spermine alkaloid Albizia stem bark
IT Albizia schimperiana
(spermine alkaloids from)
IT Alkaloids, preparation
RL: PUR (Purification or recovery); PREP (Preparation)
(spermine; from Albizia schimperiana)
IT 178494-87-6D, Budmunchiamine K, derivs.
RL: MSC (Miscellaneous)
(from Albizia schimperiana)
IT 139750-76-8P, Budmunchiamine A 178494-83-2P, 6'.xi.-Hydroxybudmunchiamine C 178494-84-3P, 5-Normethylbudmunchiamine K 178494-85-4P, 6'.xi.-Hydroxy-5-normethylbudmunchiamine K 178494-86-5P, 14-Normethylbudmunchiamine K
RL: PUR (Purification or recovery); PREP (Preparation)
(from Albizia schimperiana)

REFERENCE 7

AN 122:1057 CA
TI Screening of compounds with potential action against calcium receptors and their use in therapy of disorders of calcium metabolism
IN Nemeth, Edward F.; Brown, Edward M.; Hebert, Steven C.; Van, Wagenen

Bradford C.; Balandrin, Manuel F.; Fuller, Forrest H.; Del Mar, Eric G.
PA Brigham and Women's Hospital, Inc., USA; Nps Pharmaceuticals, Inc.
SO PCT Int. Appl., 282 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K031-00
ICS A61K031-13; A61K031-135; A61K031-405; C07K015-00; C12N015-12; C12N015-11; C12N005-10; C07K013-00; C07K015-28; A01K067-027
CC 1-1 (Pharmacology)
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9418959	A1	19940901	WO 1993-US1642	19930223
W: AT, AU, BB, BG, BR, BY, CA, CH, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, PL, RO, RU, SD, SE				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
AU 9337770	A1	19940914	AU 1993-37770	19930223
EP 637237	A1	19950208	EP 1993-907015	19930223
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 07506380	T2	19950713	JP 1993-509948	19930223
RU 2146132	C1	20000310	RU 1994-36778	19930223

PRAI WO 1993-US1642 19930223

AB A method and compn. useful for treating a patient having a disease characterized by an abnormal level of one or more components, the activity of which is regulated or affected by activity of one or more inorg.-ion receptor. Novel compds. useful in these methods and compns. are also provided. The method includes administering to the patient a therapeutically effective amt. of a mol. active at one or more inorg.-ion receptors as an agent or antagonist. Preferably, the mol. is able to act as either a selective agonist or antagonist at a Ca2+ receptor of one or more but not all cells chosen from the group consisting of parathyroid cells, bone osteoclasts, juxtaglomerular kidney cells, proximal tubule kidney cells, distal tubule kidney cell, cell of the thick ascending limb of Henle's loop and/or collecting duct, keratinocyte in the epidermis, parafollicular cell in the thyroid (C-cells), intestinal cell, trophoblast in the placenta, platelet, vascular smooth muscle cell, cardiac atrial cell, gastrin and glucagon secreting cells, kidney mesangial cell and mammary cell.

ST calcium receptor cDNA agonist antagonist screening

IT Gene, animal
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES (Uses)
(cDNA, for calcium or other inorg. ion receptor, cloning and heterologous expression of; screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT Parathyroid gland
(cell culture; in screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT Immunoassay
(for calcium receptors; in screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT Antibodies
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(for calcium receptors; in screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT Nucleic acid hybridization

(for detection of calcium receptor coding sequences; screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT Osteoclast
Trophoblast
(in screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT Xenopus laevis
(oocyte; in screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT Hyperparathyroidism
Hypertension
Osteoporosis
(screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT Thyroid gland
(C cell, in screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT Bone, disease
(Paget's, screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT Receptors
RL: BPN (Biosynthetic preparation); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(calcium, screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT Deoxyribonucleic acid sequences
(complementary, for bovine parathyroid calcium receptor)

IT Deoxyribonucleic acids
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(complementary, antisense, to calcium receptor sequences; screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT Glycerides, biological studies
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence)
(di-, in screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT Pharmaceutical dosage forms
(immunotoxins, calcium receptor-binding; screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT Kidney
(juxtaglomerular cell, in screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT Skin
(keratinocyte, in screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT Parathyroid gland
(neoplasm, inhibitors; screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT Egg
(oocyte, Xenopus laevis; in screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT Kidney
(proximal tubule, in screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium

metab.)

IT 141436-78-4, Protein kinase C
RL: MSC (Miscellaneous)
(activators; in screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT 88269-39-0, Inositol-1,4,5-trisphosphate
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence)
(in screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT 9002-64-6, Parathyroid hormone 9007-12-9, Calcitonin
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(in screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT 16561-29-8, Phorbol myristate acetate 34807-41-5, Mezerein 90365-57-4, (-)-Indolactam V
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(in screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT 7440-70-2, Calcium, biological studies
RL: ADV (Adverse effect, including toxicity); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(metabolic disorders; screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT 159480-97-4, DNA (cattle parathyroid cell clone BoPCaR1 calcium receptor cDNA and flanks)
RL: BOC (Biological occurrence); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PROC (Process); USES (Uses)
(nucleotide sequence; screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT 7439-95-4, Magnesium, biological studies
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT 7440-54-2, Gadolinium, biological studies 86933-74-6
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT 52-53-9, Verapamil 57-92-1, Streptomycin, biological studies 71-44-3, Spermine 98-84-0 112-24-3 112-57-2 119-04-0, Neomycin B 124-20-9, Spermidine 296-35-5, Hexacyclen 390-64-7 2783-17-7, 1,12-Diaminododecane 4067-16-7, Pentaethylenehexamine 4696-76-8, Bekanamycin 5966-41-6 10137-87-8 13042-18-7 13042-24-5 13042-25-6 16662-47-8 21829-25-4, Nifedipine 25104-18-1, Polylysine 25212-18-4, Polyarginine 25876-10-2, Gentamicin C1 25876-11-3, Gentamicin C2 26098-04-4, Gentamicin C1a 28075-29-8 32512-24-6 33542-87-9 38235-77-7 39562-70-4, Nitrendipine 42399-41-7, Diltiazem 57818-92-5, TMB-8 58116-20-4 71145-03-4, Bay K 8644 78005-41-1, Protamine CII (Oncorhynchus mykiss testis) 87182-56-7 87955-89-3 88976-53-8 95584-84-2 96623-89-1 97217-83-9 105029-41-2, Argiotoxin 636 108393-62-0 108448-58-4 111944-83-3, Argiotoxin 659

114753-71-8 114753-72-9 114753-78-5 114753-79-6 114753-87-6
114753-88-7 114753-89-8 115976-91-5 125275-99-2 139750-76-8,
Budmunchiamine A 148717-47-9 148717-48-0 148717-49-1 148717-50-4
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159150-05-7 159150-06-8 159150-07-9 159150-08-0 159150-09-1
159150-10-4 159150-11-5 159150-12-6 159150-13-7 159150-14-8
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159150-20-6 159150-21-7 159150-22-8 159150-23-9 159150-24-0
159150-25-1 159150-26-2 159150-27-3 159150-28-4 159150-29-5
159150-30-8 159150-31-9 159150-32-0 159150-33-1 159247-72-0
159247-73-1 159247-74-2
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT 60-92-4, CAMP
RL: BPR (Biological process); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); PROC (Process)
(screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

IT 586-37-8 2038-57-5, Benzenepropanamine
RL: RCT (Reactant); RACT (Reactant or reagent)
(screening of compds. with potential action against calcium receptors and their use in therapy of disorders of calcium metab.)

REFERENCE 8

AN 119:63054 CA
TI Calcium receptor-active molecules
IN Nemeth, Edward F.; Van Wagenen, Bradford C.; Balandrin, Manuel F.
PA NPS Pharmaceuticals, Inc., USA
SO PCT Int. Appl., 193 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM G01N033-566
ICS G01N033-567; C07C211-02; C07C211-16; C07C211-27; C07H021-00; C07K005-00; C07K007-00; C12N015-12; A61K037-02
CC 1-10 (Pharmacology)
Section cross-reference(s): 9, 63
FAN.CNT 9

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9304373	A1	19930304	WO 1992-US7175	19920821

W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, PL, RO, RU, SD, SE, US
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG

	AU 9225889	A1	19930316	AU 1992-25889	19920821
	AU 673500	B2	19961114		
	JP 06510531	T2	19941124	JP 1992-504650	19920821
	JP 2728564	B2	19980318		
	EP 657029	A1	19950614	EP 1992-919933	19920821
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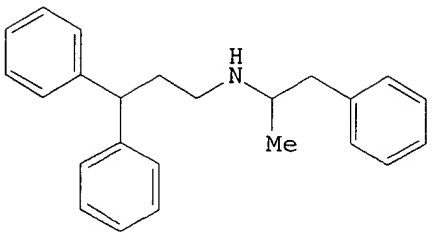
	JP 09281209	A2	19971031	JP 1996-232165	19920821
	JP 09328420	A2	19971222	JP 1996-232130	19920821
	JP 11221095	A2	19990817	JP 1998-313631	19920821
	JP 3256502	B2	20020212		
	RU 2147574	C1	20000420	RU 1994-20394	19920821
	JP 2001220356	A2	20010814	JP 2000-394979	19920821
	EP 1281702	A2	20030205	EP 2002-16612	19920821
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, IE				
	CN 1071333	A	19930428	CN 1992-111580	19920822
	CN 1067550	B	20010627		
	IL 102917	A1	20001206	IL 1992-102917	19920823
	ZA 9206360	A	19930330	ZA 1992-6360	19920824
	NO 9400581	A	19940425	NO 1994-581	19940221
	AU 9671977	A1	19970220	AU 1996-71977	19961125
	AU 711247	B2	19991007		
	AU 9931226	A1	19990722	AU 1999-31226	19990524
	AU 747853	B2	20020523	AU 1999-61707	19991126
	AU 9961707	A1	20000224		

PRAI	US 1991-749451	19910823
	US 1992-834044	19920211
	US 1992-934161	19920821
	EP 1992-919933	19920821
	JP 1992-504650	19920821
	JP 1996-232165	19920821
	JP 1998-313631	19920821
	WO 1992-US7175	19920821
	US 1993-141248	19931022
	US 1994-292827	19940819
	AU 1994-80872	19941021

GI



I

AB Methods, compns., and compds. are disclosed for treating a patient having a disease characterized by an abnormal level of component(s), the activity of which is regulated or affected by the activity of .gtoreq.1 Ca2+ receptors. The compds. act as agonists or antagonists of the Ca2+ receptors, preferably selective to receptors on parathyroid cells, bone osteoclasts, juxtaglomerular kidney cells, proximal tubule kidney cells, keratinocytes, parafollicular thyroid cells, and placental trophoblasts. A method for diagnosis of a disease comprises identifying the no. and/or location of Ca2+ receptors and making a comparison to that of normal subjects. Methods for identifying useful therapeutic mols. are also disclosed. Structure-function (intracellular Ca2+-mobilizing) studies were done on aminoglycosides and other compds. on various cells. Recombinant Ca2+ receptor protein mRNAs were expressed in Xenopus oocytes.

Compd. NPS 449 (I) caused a concn.-dependent inhibition of bone resorption with an IC50 of 10 .mu.M.

ST calcium receptor agonist antagonist

IT Blood
Blood serum
(calcium of, redn. of, by calcium receptor-active NPS 467)

IT Osteoclast
(calcium receptor on)

IT Trophoblast
(calcium receptor on, of placenta)

IT Antihypertensives
(calcium receptor-active mols.)

IT Pharmaceutical analysis
(calcium receptor-active mols. identification in, screening method for)

IT Immunoassay
(calcium receptors detn. by, for disease diagnosis)

IT Neoplasm
(diagnosis of, calcium receptors detn. in)

IT Gene, animal
RL: BIOL (Biological study)
(for calcium receptor)

IT Ribonucleic acids, messenger
RL: BIOL (Biological study)
(for exogenous calcium receptor, chloride ion conductance increase in Xenopus oocyte elicitation by)

IT Neoplasm inhibitors
(for hypercalcemia-causing tumors, calcium receptor-active mols.)

IT Protamines
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(intracellular calcium-mobilizing activity of)

IT Diagnosis
(of calcium-related diseases or conditions, calcium receptors detn. in)

IT Xenopus
Xenopus laevis
(oocytes of, chloride ion conductance increase in, exogenous calcium receptor mRNA elicitation of)

IT Parathyroid gland
(parathyroid hormone secretion by cells of, intracellular calcium levels-affecting substance inhibition of)

IT Peptides, biological studies
RL: BIOL (Biological study)
(pos.-charged, calcium receptor-active mols.)

IT Bone, metabolism
(resorption of, intracellular calcium levels-affecting substance inhibition of)

IT Antibodies
RL: BIOL (Biological study)
(to calcium receptors, for immunoassay for disease diagnosis)

IT Osteoporosis
(treatment of, with calcium receptor-active mols.)

IT Placenta
(trophoblasts of, calcium receptor on)

IT Thyroid gland, composition
(C cell, calcium receptor on)

IT Bone, disease
(Paget's, treatment of, with calcium receptor-active mols.)

IT Amines, biological studies
RL: BIOL (Biological study)
(alkaryl, calcium receptor-active mols.)

IT Glycosides
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); BIOL (Biological study)
(amino, intracellular calcium-mobilizing activity of)

IT Polyamines
RL: BIOL (Biological study)
(branched, calcium receptor-active mols.)

IT Ion channel blockers
Ion channel openers
(calcium, pharmaceuticals)

IT Receptors
RL: BIOL (Biological study)
(calcium, substances binding and active with, of osteoclasts and other cells)

IT Molecular structure-biological activity relationship
(calcium-mobilizing, intracellular, of aminoglycosides and other polyamines)

IT Glycerides, biological studies
RL: BIOL (Biological study)
(di-, intracellular calcium levels-affecting substance causing increase in)

IT Kidney, composition
(juxtaglomerular cell, calcium receptor on)

IT Skin, composition
(keratinocyte, calcium receptor on)

IT Parathyroid gland
(neoplasm, diagnosis of, calcium receptors detn. in)

IT Egg
(oocyte, chloride ion conductance increase in, of Xenopus, exogenous calcium receptor mRNA elicitation of)

IT Pharmaceutical dosage forms
(oral, of calcium receptor-active NPS 467 isomer, blood serum calcium lowering with)

IT Amines, biological studies
RL: BIOL (Biological study)
(poly-, cyclic, calcium receptor-active mols.)

IT Hyperparathyroidism
(primary, treatment of, with calcium receptor-active mols.)

IT Kidney, composition
(proximal tubule, calcium receptor on cell of)

IT Hyperparathyroidism
(secondary, treatment of, with calcium receptor-active mols.)

IT Biological transport
(translocation, of intracellular calcium, calcium receptor-active substances effect on)

IT 51-61-6, Dopamine, biological studies 7683-59-2, Isoproterenol
RL: BIOL (Biological study)
(cAMP formation stimulated by, intracellular calcium levels-affecting substance inhibition of)

IT 148740-51-6
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(calcilytic activity of, on parathyroid cells)

IT 390-64-7 13042-18-7 108448-58-4 114753-78-5 133805-32-0 148717-48-0 148717-50-4
RL: BIOL (Biological study)
(calcium receptor-active mol.)

IT 108393-62-0D, derivs.
RL: BIOL (Biological study)
(calcium receptor-active mols.)

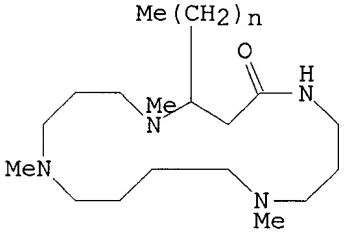
IT 16887-00-6, Chloride ion, biological studies
RL: PRP (Properties)
(conductance of, increase in, in Xenopus oocytes injected with mRNA for calcium receptor)

IT 60-92-4, CAMP
RL: FORM (Formation, nonpreparative)
(formation of, dopamine- or isoproterenol-stimulated, intracellular calcium levels-affecting substance inhibition of)
IT 16561-29-8, Phorbol myristate acetate 34807-41-5, Mezerein 90365-57-4, (-)-Indolactam V
RL: BIOL (Biological study)
(intracellular calcium levels-affecting substance activity inhibition by)
IT 141436-78-4, Protein kinase C
RL: BIOL (Biological study)
(intracellular calcium levels-affecting substance activity inhibition by activator of)
IT 88269-39-0, Inositol-1,4,5-triphosphate
RL: BIOL (Biological study)
(intracellular calcium levels-affecting substance causing increase in)
IT 7681-49-4, Sodium fluoride, biological studies
RL: BIOL (Biological study)
(intracellular calcium levels-affecting substance inhibition by)
IT 7439-96-5, Manganese, biological studies
RL: BIOL (Biological study)
(intracellular calcium-mobilizing activity of)
IT 52-53-9 57-92-1, Streptomycin, biological studies 71-44-3, Spermine 112-24-3, Triethylenetetramine 112-57-2, Tetraethylenepentamine 119-04-0, Neomycin B 124-20-9, Spermidine 154-21-2, Lincomycin 296-35-5, Hexacyclen 1403-66-3, Gentamicin 2783-17-7, 1,12-Diaminododecane 4067-16-7, Pentaethylenehexamine 4696-76-8, Bekanamycin 8063-07-8, Kanamycin 16662-47-8 24937-47-1 25104-18-1 25212-18-4 38000-06-5 42399-41-7, Diltiazem 57818-92-5, TMB-8 87955-89-3 105029-41-2, Argiotoxin 636 111944-83-3, Argiotoxin 659 115976-91-5, Philanthotoxin 433 128549-96-2, Agatoxin 489 128549-97-3 139750-76-8, Budmunchiamine A 148717-51-5 148717-52-6 148717-53-7 148740-50-5
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(intracellular calcium-mobilizing activity of)
IT 159149-75-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of and bovine parathyroid cell calcium receptor activation by)
IT 148717-54-8P 148717-55-9P 148717-56-0P 148740-52-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of and bovine parathyroid cell calcium receptor activation by)
IT 148717-47-9P 148717-49-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of and calcium receptor activity of)
IT 13042-18-7DP, Fendiline, analogs 13042-18-7P, Fendiline
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, calcium receptor-active substances in relation to)
IT 5586-73-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with acetophenone, in prepn. of calcium receptor-active substance)
IT 98-86-2, Acetophenone, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with bisphenylpropylamine, in prepn. of calcium receptor-active substance)
IT 2038-57-5, 3-Phenylpropylamine 18655-48-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methoxyacetophenone)
IT 586-37-8, 3'-Methoxyacetophenone

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phenylpropylamine)
IT 9002-64-6, Parathyroid hormone
RL: BIOL (Biological study)
(secretion of, by parathyroid cell, intracellular calcium levels-affecting substance inhibition of)
IT 9007-12-9, Calcitonin
RL: BIOL (Biological study)
(secretion of, stimulation of, with calcium receptor-binding substance)
IT 7440-70-2, Calcium, biological studies
RL: BIOL (Biological study)
(substances increasing or blocking intracellular)

REFERENCE 9

AN 117:23236 CA
TI DNA-based isolation and the structure elucidation of the budmunchiamines, novel macrocyclic alkaloids from Albizia amara
AU Pezzuto, John M.; Mar, Woongchon; Lin, Long Ze; Cordell, Geoffrey A.; Neszmelyi, Andras; Wagner, Hildebert
CS Coll. Pharm., Univ. Illinois, Chicago, IL, USA
SO Heterocycles (1991), 32(10), 1961-7
CODEN: HTCYAM; ISSN: 0385-5414
DT Journal
LA English
CC 11-1 (Plant Biochemistry)
Section cross-reference(s): 31
GI



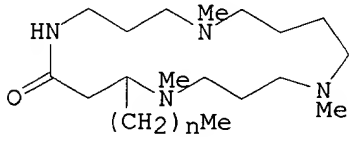
I, n=10
II, n=8
III, n=12

AB On the basis of DNA affinity, a novel isolate was obtained from an ext. prepd. from the seeds of A. amara. As detd. by a series of spectroscopic techniques, the isolate was structurally defined as a mixt. of 3 macrocyclic alkaloids of the pithecolobine type that differed only in the length of the aliph. side chain. The 1H- and 13C-NMR spectral parameters were unambiguously assigned to these alkaloids, which were given the trivial names budmunchiamine A (I), B (II), or C (III). With the exception of former studies performed with Pithecolobium saman, this is the only other reported of pithecolobine alkaloids being found in nature.
ST Albizia pithecolobine alkaloid budmunchiamine
IT Nomenclature, new natural products
(budmunchiamine A (alkaloid))
IT Nomenclature, new natural products
(budmunchiamine B (alkaloid))
IT Nomenclature, new natural products
(budmunchiamine C (alkaloid))
IT Albizia amara
(macrocyclic alkaloids from, structure of)
IT Molecular structure, natural product
(of budmunchiamine A (alkaloid))
IT Molecular structure, natural product

(of budmunchiamine B (alkaloid))
IT Molecular structure, natural product
(of budmunchiamine C (alkaloid))
IT Alkaloids, biological studies
RL: BIOL (Biological study)
(macrocyclic, pithecolobine, from Albizia amara)
IT 139750-76-8, Budmunchiamine A 139750-77-9, Budmunchiamine B 139750-78-0, Budmunchiamine C
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of Albizia amara, isolation and structure detn. of)

REFERENCE 10

AN 116:207412 CA
TI Biological activity of novel macrocyclic alkaloids (budmunchiamines) from Albizia amara detected on the basis of interaction with DNA
AU Mar, Woongchon; Tan, Ghee T.; Cordell, Geoffrey A.; Pezzuto, John M.; Jurcic, Ksenija; Offermann, Franziska; Redl, Karl; Steinke, Bernice; Wagner, Hildebert
CS Coll. Pharm, Univ. Illinois, Chicago, IL, 60612, USA
SO Journal of Natural Products (1991), 54(6), 1531-42
CODEN: JNPRDF; ISSN: 0163-3864
DT Journal
LA English
CC 1-6 (Pharmacology)
GI



I, n=10
II, n=8
III, n=12

AB Exts. derived from A. amara were found to demonstrate activity in a recently developed HPLC system designed to detect compds. capable of interacting with DNA. Further investigation led to the procurement of four sets of alkaloid isolates X1-X4 that were found to be macrocyclic pithecolobine alkaloids. Isolate X1 has been identified as a mixt. of budmunchiamines A, B, and C (I, II, and III) in the ratio 4:4:1. All four isolates interacted with calf thymus DNA and were generally cytotoxic with a battery of cultured mammalian cells. As detd. with Salmonella typhimurium strain TM677, isolates X1 and X3 were bactericidal, but not mutagenic. Isolate X1 was found to inhibit the catalytic activity of DNA polymerase, RNA polymerase, and HIV-1 reverse transcriptase. With DNA polymerase, the reaction was shown to be inhibited in a manner that was competitive with respect to DNA. In addn., isolate X1 inhibited each of the following: platelet aggregation, human lymphocyte transformation, phorbol-ester-induced chemiluminescence with human granulocytes, and cyclooxygenase activity. Detection of these alkaloids on the basis of their interaction with DNA exemplifies the validity of this approach.
ST Albizia pithecolobine alkaloid budmunchiamine DNA pharmacol
IT Albizia amara
(alkaloids of, budmunchiamines-contg., DNA-interaction as index for isolation of, pharmacol. of)
IT Antibiotics
Blood platelet aggregation inhibitors
Inflammation inhibitors
Mutagens

Neoplasm inhibitors
(budmunchiamines-contg. alkaloids from Albizia amara as, DNA-interaction as index for isolation of)

IT Deoxyribonucleic acids
RL: BIOL (Biological study)
(interaction with, as index for isolation of budmunchiamines-contg. alkaloids from Albizia amara, pharmacol. of)

IT Alkaloids, biological studies
RL: BIOL (Biological study)
(of Albizia amara, budmunchiamines-contg., DNA-interaction as index for isolation of, pharmacol. of)

IT Luminescence, chemi-
(with human granulocyte, budmunchiamines-contg. alkaloids from Albizia amara effect on, DNA-interaction as index of, antiinflammatory action in relation to)

IT Leukocyte
(granulocyte, chemiluminescence with human, budmunchiamines-contg. alkaloids from Albizia amara effect on, DNA-interaction as index of, antiinflammatory action in relation to)

IT Virus, animal
(human immunodeficiency 1, reverse transcriptase of, budmunchiamines-contg. alkaloids from Albizia amara effect on, DNA-interaction as index of)

IT 9012-90-2, DNA polymerase 9014-24-8, RNA polymerase
RL: BIOL (Biological study)
(budmunchiamines-contg. alkaloids from Albizia amara effect on, DNA-interaction as index of)

IT 39391-18-9, Cyclooxygenase
RL: BIOL (Biological study)
(budmunchiamines-contg. alkaloids from Albizia amara effect on, DNA-interaction as index of, anti-inflammatory action in relation to)

IT 9068-38-6, Reverse transcriptase
RL: BIOL (Biological study)
(of HIV-1, budmunchiamines-contg. alkaloids from Albizia amara effect on, DNA-interaction as index of)

IT 139750-76-8, Budmunchiamine A 139750-77-9, Budmunchiamine B 139750-78-0, Budmunchiamine C
RL: BIOL (Biological study)
(Albizia amara alkaloids contg., DNA-interaction as index for isolation of, pharmacol. of)

=> d is
'IS' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN
SAM - Index Name, MF, and structure - no RN
FIDE - All substance data, except sequence data
IDE - FIDE, but only 50 names
SQIDE - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD - Protein sequence data, includes RN
SQD3 - Same as SQD, but 3-letter amino acid codes are used
SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties

```
EPROP  - Table of experimental properties
PROP   - EPROP and CALC

Any CA File format may be combined with any substance format to
obtain CA references citing the substance.  The substance formats
must be cited first.  The CA File predefined formats are:

ABS  -- Abstract
APPS -- Application and Priority Information
BIB  -- CA Accession Number, plus Bibliographic Data
CAN  -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND  -- Index Data
IPC  -- International Patent Classification
PATS -- PI, SO
STD  -- BIB, IPC, and NCL

IABS --ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when
it is available.
The MAX format is the same as ALL.
The IALL format is the same as ALL with BIB ABS and IND indented,
with text labels.

For additional information, please consult the following help
messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):d his
'D' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
'HIS' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual
fields or predefined formats.  The predefined substance formats
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SQD    - Protein sequence data, includes RN
SQD3   - Same as SQD, but 3-letter amino acid codes are used
SQN    - Protein sequence name information, includes RN

CALC   - Table of calculated properties
EPROP  - Table of experimental properties
PROP   - EPROP and CALC
```

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

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ISTD -- STD format, indented

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OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.
The MAX format is the same as ALL.
The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):bib
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The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN
SAM - Index Name, MF, and structure - no RN
FIDE - All substance data, except sequence data
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SQIDE - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD - Protein sequence data, includes RN
SQD3 - Same as SQD, but 3-letter amino acid codes are used
SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties
EPROP - Table of experimental properties
PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

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CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND -- Index Data
IPC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IPC, and NCL

IABS --ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when
it is available.
The MAX format is the same as ALL.
The IALL format is the same as ALL with BIB ABS and IND indented,
with text labels.

For additional information, please consult the following help
messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):ide

L11 ANSWER 1 OF 22 REGISTRY COPYRIGHT 2003 ACS
RN   195734-30-6 REGISTRY
CN   1,5,9,13-Tetraazacycloheptadecan-6-one, 8-(11-pentadecenyl)-, (+)- (9CI)
     (CA INDEX NAME)
OTHER NAMES:
CN   **(+)-Budmunchiamine L6**
CN   **Budmunchiamine L 6**
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MF   C28 H56 N4 O
SR   CA
LC   STN Files: CA, CAPLUS

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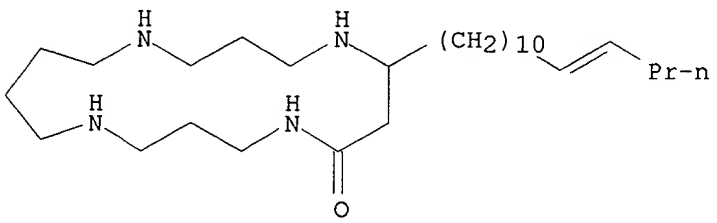

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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L3             0 S L1 EXA SAM
L4             0 S L1 FAM SAM
L5             2 S L1 SSS SAM
L6               STRUCTURE UPLOADED
L7               QUE L6
L8             2 S L6 SSS FULL
                 E SPERMI
                 E SPERMIDINE
L9          2411 S E3
                 E SPERMINE
L10          262 S E3-E4
                 E BUDMUNCHIMINE
L11           22 S E1-E2

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COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                     ENTRY    SESSION
FULL ESTIMATED COST                                 265.24     265.45

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)      SINCE FILE      TOTAL
                                                     ENTRY    SESSION
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FILE COVERS 1907 - 18 Mar 2003  VOL 138 ISS 12
FILE LAST UPDATED: 17 Mar 2003  (20030317/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> d his

     (FILE 'HOME' ENTERED AT 12:58:18 ON 18 MAR 2003)

     FILE 'REGISTRY' ENTERED AT 12:58:26 ON 18 MAR 2003
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L1              STRUCTURE UPLOADED
L2              QUE L1
L3            0 S L1 EXA SAM
L4            0 S L1 FAM SAM
L5            2 S L1 SSS SAM
L6              STRUCTURE UPLOADED
L7              QUE L6
L8            2 S L6 SSS FULL
                E SPERMI
                E SPERMIDINE
L9         2411 S E3
                E SPERMINE
L10         262 S E3-E4
                E BUDMUNCHIMINE
L11          22 S E1-E2

     FILE 'CAPLUS' ENTERED AT 13:34:14 ON 18 MAR 2003

=> e cancer
E1           13     CANCENTRINE/BI
E2            1     CANCENTRINEMETHINE/BI
E3       182103 --> CANCER/BI
E4            1     CANCER0/BI
E5            4     CANCER1/BI
E6            1     CANCER10/BI
E7            1     CANCER4/BI
E8            1     CANCERA/BI
E9            2     CANCERAND/BI
E10           1     CANCERARRAY/BI
E11          35     CANCERATION/BI
E12           1     CANCERB/BI

=> s e3
L12      182103 CANCER/BI

=> s l12 and l11
            13 L11
L13          1 L12 AND L11

=> d l13 1

L13  ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2003 ACS
AN   2002:107323  CAPLUS
DN   136:167548
TI   Synthesis of cyclic polyamine analogs for cancer therapy
IN   Frydman, Benjamin; Hesse, Manfred; Guggisberg, Armin; Popaj, Kasmin;
     Drandarov, Konstantin; Basu, Hirak; Bhattacharya, Subhra; Wang, Yu
PA   Slil Biomedical Corporation, USA
SO   PCT Int. Appl., 105 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
     ---------------   ----  --------       ---------------  --------
PI   WO 2002010142      A1   20020207       WO 2001-US24282  20010802
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT,
             RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US,
             UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
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        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
            DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
            BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
PRAI US 2000-222522P   P    20000802
OS   MARPAT 136:167548
RE.CNT  2     THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
              ALL CITATIONS AVAILABLE IN THE RE FORMAT


=> e neoplastic
E1            1     NEOPLASTC/BI
E2            2     NEOPLASTIA/BI
E3        41765 --> NEOPLASTIC/BI
E4            2     NEOPLASTICA/BI
E5          333     NEOPLASTICALLY/BI
E6            1     NEOPLASTICCELL/BI
E7            1     NEOPLASTICDISEASES/BI
E8            8     NEOPLASTICITY/BI
E9            1     NEOPLASTICLLY/BI
E10           3     NEOPLASTICLY/BI
E11           1     NEOPLASTICO/BI
E12           1     NEOPLASTICPROCESS/BI

=> s e3
L14       41765 NEOPLASTIC/BI

=> s l14 and l11
             13 L11
L15           0 L14 AND L11

=> e parasite
E1            1     PARASITCIDAL/BI
E2            2     PARASITCUS/BI
E3        21796 --> PARASITE/BI
E4            3     PARASITED/BI
E5            1     PARASITEES/BI
E6            1     PARASITEFREE/BI
E7            1     PARASITEHOST/BI
E8            1     PARASITEINFECTED/BI
E9           18     PARASITELLA/BI
E10        1624     PARASITEMIA/BI
E11           1     PARASITEMIAIN/BI
E12         232     PARASITEMIAS/BI

=> s e1-e12
              1 PARASITCIDAL/BI
              2 PARASITCUS/BI
          21796 PARASITE/BI
              3 PARASITED/BI
              1 PARASITEES/BI
              1 PARASITEFREE/BI
              1 PARASITEHOST/BI
              1 PARASITEINFECTED/BI
             18 PARASITELLA/BI
           1624 PARASITEMIA/BI
              1 PARASITEMIAIN/BI
            232 PARASITEMIAS/BI
L16       22877 (PARASITCIDAL/BI OR PARASITCUS/BI OR PARASITE/BI OR PARASITED/BI
                 OR PARASITEES/BI OR PARASITEFREE/BI OR PARASITEHOST/BI OR PARAS
                ITEINFECTED/BI OR PARASITELLA/BI OR PARASITEMIA/BI OR PARASITEMI
                AIN/BI OR PARASITEMIAS/BI)
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```
=> s l16 and l11
            13 L11
L17          0 L16 AND L11

=> s antiviral or hiv or herpes or hsv or viral
         37643 ANTIVIRAL
         48320 HIV
         21125 HERPES
          9356 HSV
        117115 VIRAL
L18     182510 ANTIVIRAL OR HIV OR HERPES OR HSV OR VIRAL

=> s l18 and l11
            13 L11
L19          1 L18 AND L11

=> d l19 1

L19  ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2003 ACS
AN   1992:207412  CAPLUS
DN   116:207412
TI   Biological activity of novel macrocyclic alkaloids (budmunchiamines) from
     Albizia amara detected on the basis of interaction with DNA
AU   Mar, Woongchon; Tan, Ghee T.; Cordell, Geoffrey A.; Pezzuto, John M.;
     Jurcic, Ksenija; Offermann, Franziska; Redl, Karl; Steinke, Bernice;
     Wagner, Hildebert
CS   Coll. Pharm, Univ. Illinois, Chicago, IL, 60612, USA
SO   Journal of Natural Products (1991), 54(6), 1531-42
     CODEN: JNPRDF; ISSN: 0163-3864
DT   Journal
LA   English


=> d l19 all

L19  ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2003 ACS
AN   1992:207412  CAPLUS
DN   116:207412
TI   Biological activity of novel macrocyclic alkaloids (budmunchiamines) from
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     Wagner, Hildebert
CS   Coll. Pharm, Univ. Illinois, Chicago, IL, 60612, USA
SO   Journal of Natural Products (1991), 54(6), 1531-42
     CODEN: JNPRDF; ISSN: 0163-3864
DT   Journal
LA   English
CC   1-6 (Pharmacology)
GI
```

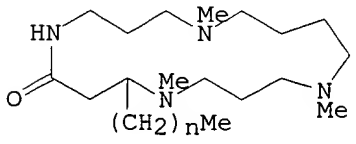

I, n=10
II, n=8
III, n=12

AB Exts. derived from A. amara were found to demonstrate activity in a recently developed HPLC system designed to detect compds. capable of interacting with DNA. Further investigation led to the procurement of four sets of alkaloid isolates X1-X4 that were found to be macrocyclic pithecolobine alkaloids. Isolate X1 has been identified as a mixt. of budmunchiamines A, B, and C (I, II, and III) in the ratio 4:4:1. All four isolates interacted with calf thymus DNA and were generally cytotoxic with a battery of cultured mammalian cells. As detd. with Salmonella typhimurium strain TM677, isolates X1 and X3 were bactericidal, but not mutagenic. Isolate X1 was found to inhibit the catalytic activity of DNA polymerase, RNA polymerase, and **HIV**-1 reverse transcriptase. With DNA polymerase, the reaction was shown to be inhibited in a manner that was competitive with respect to DNA. In addn., isolate X1 inhibited each of the following: platelet aggregation, human lymphocyte transformation, phorbol-ester-induced chemiluminescence with human granulocytes, and cyclooxygenase activity. Detection of these alkaloids on the basis of their interaction with DNA exemplifies the validity of this approach.

ST Albizia pithecolobine alkaloid budmunchiamine DNA pharmacol

IT Albizia amara
(alkaloids of, budmunchiamines-contg., DNA-interaction as index for isolation of, pharmacol. of)

IT Antibiotics
Blood platelet aggregation inhibitors
Inflammation inhibitors
Mutagens
Neoplasm inhibitors
(budmunchiamines-contg. alkaloids from Albizia amara as, DNA-interaction as index for isolation of)

IT Deoxyribonucleic acids
RL: BIOL (Biological study)
(interaction with, as index for isolation of budmunchiamines-contg. alkaloids from Albizia amara, pharmacol. of)

IT Alkaloids, biological studies
RL: BIOL (Biological study)
(of Albizia amara, budmunchiamines-contg., DNA-interaction as index for isolation of, pharmacol. of)

IT Luminescence, chemi-
(with human granulocyte, budmunchiamines-contg. alkaloids from Albizia amara effect on, DNA-interaction as index of, antiinflammatory action in relation to)

IT Leukocyte
(granulocyte, chemiluminescence with human, budmunchiamines-contg. alkaloids from Albizia amara effect on, DNA-interaction as index of, antiinflammatory action in relation to)

IT Virus, animal
(human immunodeficiency 1, reverse transcriptase of, budmunchiamines-contg. alkaloids from Albizia amara effect on, DNA-interaction as index of)

IT 9012-90-2, DNA polymerase 9014-24-8, RNA polymerase
RL: BIOL (Biological study)
(budmunchiamines-contg. alkaloids from Albizia amara effect on, DNA-interaction as index of)

IT 39391-18-9, Cyclooxygenase
RL: BIOL (Biological study)
(budmunchiamines-contg. alkaloids from Albizia amara effect on, DNA-interaction as index of, anti-inflammatory action in relation to)

IT 9068-38-6, Reverse transcriptase
RL: BIOL (Biological study)
(of **HIV**-1, budmunchiamines-contg. alkaloids from Albizia amara effect on, DNA-interaction as index of)

IT **139750-76-8**, Budmunchiamine A **139750-77-9**,

Budmunchiamine B **139750-78-0**, Budmunchiamine C
RL: BIOL (Biological study)
(Albizia amara alkaloids contg., DNA-interaction as index for isolation of, pharmacol. of)

=> d his

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L1 STRUCTURE UPLOADED
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L3 0 S L1 EXA SAM
L4 0 S L1 FAM SAM
L5 2 S L1 SSS SAM
L6 STRUCTURE UPLOADED
L7 QUE L6
L8 2 S L6 SSS FULL
E SPERMI
E SPERMIDINE
L9 2411 S E3
E SPERMINE
L10 262 S E3-E4
E BUDMUNCHIMINE
L11 22 S E1-E2

FILE 'CAPLUS' ENTERED AT 13:34:14 ON 18 MAR 2003
E CANCER
L12 182103 S E3
L13 1 S L12 AND L11
E NEOPLASTIC
L14 41765 S E3
L15 0 S L14 AND L11
E PARASITE
L16 22877 S E1-E12
L17 0 S L16 AND L11
L18 182510 S ANTIVIRAL OR HIV OR HERPES OR HSV OR VIRAL
L19 1 S L18 AND L11

=>

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=>
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=> LOG Y

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